

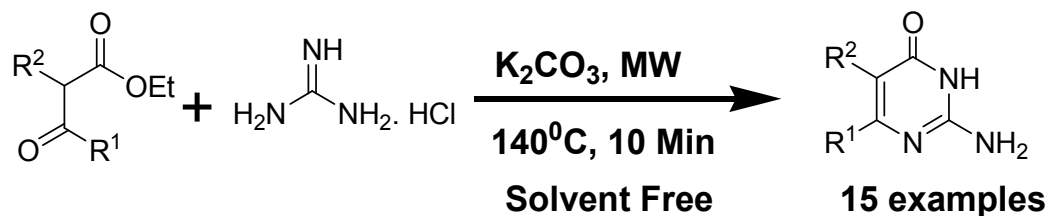
## Supporting information

### Direct synthesis of 5- and 6- substituted 2-aminopyrimidines as potential non-natural nucleobase analogues

K. Radhakrishnan, Namita Sharma and Lal Mohan Kundu\*

Department of Chemistry, Indian Institute of Technology Guwahati, North Guwahati, Assam-781039, India.

\*Corresponding author Fax: + 91 361 2582349; Tel: +91 361 2582326; E-mail: [lmkundu@iitg.ernet.in](mailto:lmkundu@iitg.ernet.in)



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III. Characterization (<sup>1</sup>H NMR and XRD data)

### I. General Information:

Chemicals used for these experiments were purchased from merck, spectrochem, and sigma Aldrich and were used as such. *CEM Discover LabMate* closed vessel microwave reactor was used to carry out all reactions. All the NMR spectra were recorded from *DRX-400 Varian* and 600 MHz *Brucker* NMR spectrometers using DMSO-*d*<sub>6</sub> and CDCl<sub>3</sub> as solvents. Melting points were obtained from *Buchi-B 545* instrument. HRMS was analyzed from *Agilent Q-TOF 6500* LC/MS system. All crystal data were obtained from *Brucker SMART APEX* equipped with a CCD area detector using Mo. The structure was solved by direct method using *SHELLX-97* (Göttingen, Germany).

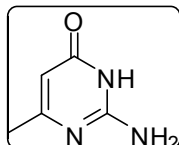
All the substrate β-ketoesters or β-aldehydoesters (**1a-15a**, as in table-1 in main text) were either purchased from reputed companies or were synthesized following published procedures.<sup>1-4</sup>

### II. General procedure:

Ester (2 mmol), guanidine hydrochloride (4 mmol) and potassium carbonate (2 mmol) were taken in a microwave reactor vessel and was closed immediately. The vessel was subjected to microwave irradiation for 10 minutes at 140 °C. The reaction vessel was allowed to cool, and the products were isolated. The desired compounds (**1-15**) were further purified by column chromatography using methanol/chloroform.

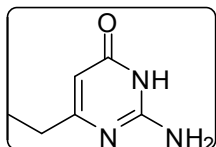
### III. Characterization part

#### 1. 2-amino-6-methylpyrimidin-4(3H)-one.



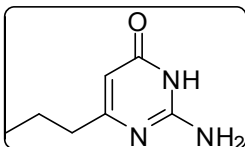
White solid, m.p 280 °C (lit<sup>5</sup> 285). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.82 (br, 1H), 6.55 (br, 2H), 5.39 (s, 1H), 1.97 (s, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 155.91, 100.81, 23.05. HRMS (ES): Calcd for C<sub>5</sub>H<sub>7</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 126.0662, found 126.0662.

#### 2. 2-amino-6-ethylpyrimidin-4(3H)-one.



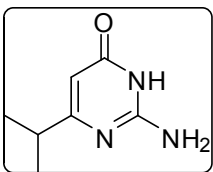
White solid, m.p 249 °C (lit<sup>6</sup> 247). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.80 (br, 1H), 6.58 (br, 2H), 5.39 (s, 1H), 2.26 (q, J=7.2Hz, 2H), 1.07 (t, J=7.3Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 167.48, 156.69, 100.54, 29.60, 13.02. HRMS (ES): Calcd for C<sub>6</sub>H<sub>9</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 140.0818, found 140.0814

#### 3. 2-amino-6-propylpyrimidin-4(3H)-one



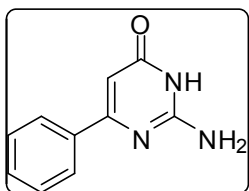
White solid, m.p 254 °C <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.74 (br, 1H), 6.48 (br, 2H), 5.37 (s, 1H), 2.20 (t, J=7Hz, 2H), 1.49-1.58 (m, 2H), 0.85 (t, J=7.2Hz, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 155.95, 100.11, 38.17, 20.77, 13.55. HRMS (ES): calcd for C<sub>7</sub>H<sub>11</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 154.0975, found 154.0976

#### 4. 2-amino-6-isopropylpyrimidin-4(3H)-one



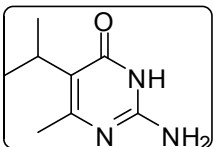
White solid, m.p 243 °C (lit<sup>7</sup> 248). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.75 (br, 1H), 6.53 (br, 2H), 5.37 (s, 1H), 2.42-2.51 (m, 1H), 1.07 (d, J=6.8Hz, 6H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 156.11, 97.82, 34.52, 21.12. HRMS (ES): Calcd for C<sub>7</sub>H<sub>11</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 154.0975, Found 154.0976

#### 5. 2-amino-6-phenylpyrimidin-4(3H)-one



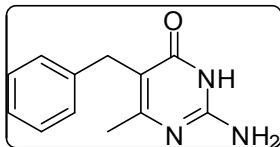
White solid, m.p 272 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.82 (br, 1H), 7.92 (br, 2H), 7.43 (br, 3H), 6.60 (br, 2H), 6.09 (s, 1H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 164.10, 155.95, 137.24, 130.15, 128.55, 126.81, 97.84. HRMS (ES): Calcd for C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 188.0818, found 188.0818

#### 6. 2-amino-5-isopropyl-6-methylpyrimidin-4(3H)-one



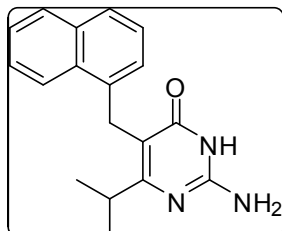
White solid, m.p 280 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.74 (br, 1H), 6.32 (br, 2H), 2.84-2.91 (m, 1H), 2.05 (s, 3H), 1.16 (d, J=7Hz, 6H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 154.29, 118.61, 27.04, 21.21, 21.00. HRMS (ES): Calcd for C<sub>8</sub>H<sub>13</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 168.1131, found 168.1125

#### 7. 2-amino-5-benzyl-6-methylpyrimidin-4(3H)-one



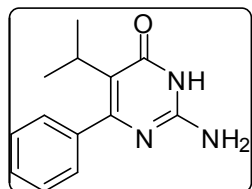
White solid, m.p 226 °C (lit<sup>8</sup> 216). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.90 (br, 1H), 7.10-7.24 (m, 5H), 6.38 (br, 2H), 3.63 (s, 2H), 2.00 (s, 3H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 154.39, 141.83, 128.80, 128.56, 126.18, 111.14, 30.53. HRMS (ES): Calcd for C<sub>12</sub>H<sub>13</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 216.1131, found 216.1131

### 8. 2-amino-6-isopropyl-5-(naphthalen-1-ylmethyl)pyrimidin-4(3H)-one



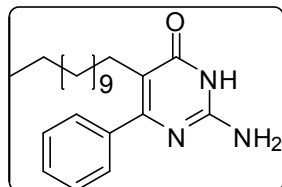
White solid, m.p 289 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.76 (br, 1H), 8.23 (d, J=8.72, 1H), 7.91 (d, J=7.84, 1H), 7.73 (d, J=8.7Hz, 1H), 7.41 (t, J=8.3Hz, 2H), 7.22 (t, J=7.4Hz, 2H), 6.47 (br, 2H), 4.12 (s, 2H), 2.74 (m, 1H), 1.07 (d, J=6.6Hz, 3H), 0.93 (d, J=5.8Hz, 3H). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>+ DMSO-*d*<sub>6</sub>): δ 155.11, 135.76, 133.24, 131.75, 128.19, 126.06, 125.44, 125.13, 123.37, 123.04, 26.32, 20.20. HRMS (ES): Calcd for C<sub>18</sub>H<sub>19</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 294.1601, found 294.1602

### 9. 2-amino-5-isopropyl-6-phenylpyrimidin-4(3H)-one



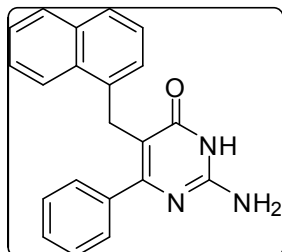
White solid, m.p 260 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.85 (br, 1H), 7.28-7.42 (m, 5H), 6.32 (br, 2H), 2.58-2.61 (m, 1H), 1.14-1.18 (d, J=6.9Hz, 6H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 153.47, 128.30, 127.99, 127.77, 126.67, 116.30, 27.83, 20.45. HRMS (ES): Calcd for C<sub>13</sub>H<sub>15</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 230.1288, found 230.1289

### 10. 2-amino-5-dodecyl-6-phenylpyrimidin-4(3H)-one



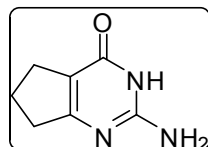
White solid, m.p 292 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.88 (br, 1H), 7.33-7.37 (m, 5H), 6.32 (br, 2H), 2.17 (t, J=7.6Hz, 2H), 1.08-1.29 (m, 20H), 0.84 (t, J=5.6Hz, 3H). HRMS (ES): Calcd for C<sub>22</sub>H<sub>33</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 356.2696, found 356.2696

### 11. 2-amino-5-(naphthalen-1-ylmethyl)-6-phenylpyrimidin-4(3H)-one



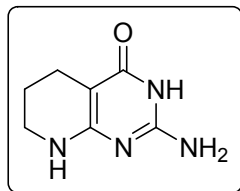
White solid, m.p >300 °C. <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 11.00 (br, 1H), 7.98 (d, J=7.2Hz, 1H), 7.90 (d, J=7.6Hz, 1H), 7.73 (d, J=8Hz, 1H), 7.47 (m, 2H), 7.35 (m, 3H), 7.25 (m, 3H), 7.08 (d, J=6.8Hz, 1H), 6.59 (br, 2H), 4.01 (s, 2H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 154.01, 136.73, 133.32, 131.56, 128.53, 127.90, 127.69, 126.19, 125.94, 125.66, 125.61, 124.10, 123.40, 108.91, 28.59. HRMS (ES): Calcd for C<sub>21</sub>H<sub>17</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 328.1444, found 328.1443

### 12. 2-amino-6,7-dihydro-3H-cyclopenta[d]pyrimidin-4(5H)-one



White solid, m.p > 300 °C (lit<sup>9</sup> >300). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.60 (br, 1H), 6.43 (br, 2H), 2.46-2.52 (m, 4H), 1.85 1.94 (m, 2H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ 161.22, 158.29, 156.27, 110.84, 34.42, 26.62, 20.96. HRMS (ES): Calcd for C<sub>7</sub>H<sub>9</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 152.0818, found 152.0814

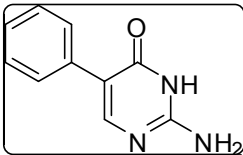
### 13. 2-amino-5,6,7,8-tetrahydropyrido[2,3-d]pyrimidin-4(3H)-one



White solid, m.p 274 °C (lit<sup>10</sup> 260) <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 9.72 (br, 1H), 6.21 (br, 1H), 5.94 (br, 2H), 3.10 (br, 2H), 2.20 (t, J=6Hz, 2H), 1.61-1.66 (m, 2H). <sup>13</sup>C NMR (100 MHz, DMSO-*d*<sub>6</sub>): δ

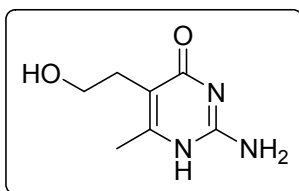
161.36, 159.68, 153.26, 82.55, 21.17, 19.17. HRMS (ES): Calcd for C<sub>7</sub>H<sub>10</sub>N<sub>4</sub>O [M+H]<sup>+</sup> 167.0927 found 167.0928

#### 14. 2-amino-5-phenylpyrimidin-4(3H)-one



White solid, m.p 240 °C (lit<sup>11</sup> 244). <sup>1</sup>H NMR (400 MHz, DMSO-*d*<sub>6</sub>): δ 10.84 (br, 1H), 7.12-7.28 (m, 5H), 6.34 (br, 2H), 3.49 (s, 1H). HRMS (ES): Calcd for C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>O [M+H]<sup>+</sup> 188.0818, found 188.0824

#### 15. 2-amino-5-(2-hydroxyethyl)-6-methylpyrimidin-4(1H)-one



White solid. m.p. 256 °C (lit<sup>12</sup> 265); <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>): δ 7.04 (s, 1H), 6.58 (br, 2H), 4.53 (br, 1H), 3.35 (t, J=7.2, 2H), 2.43 (t, J=7.2, 2H), 2.06 (s, 3H). <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>): δ 164.52, 158.12, 153.43, 108.34, 60.00, 28.81, 20.53. HRMS (ES): Calcd for C<sub>7</sub>H<sub>11</sub>N<sub>3</sub>O<sub>2</sub> [M+H]<sup>+</sup> 170.0924, found 170.0928

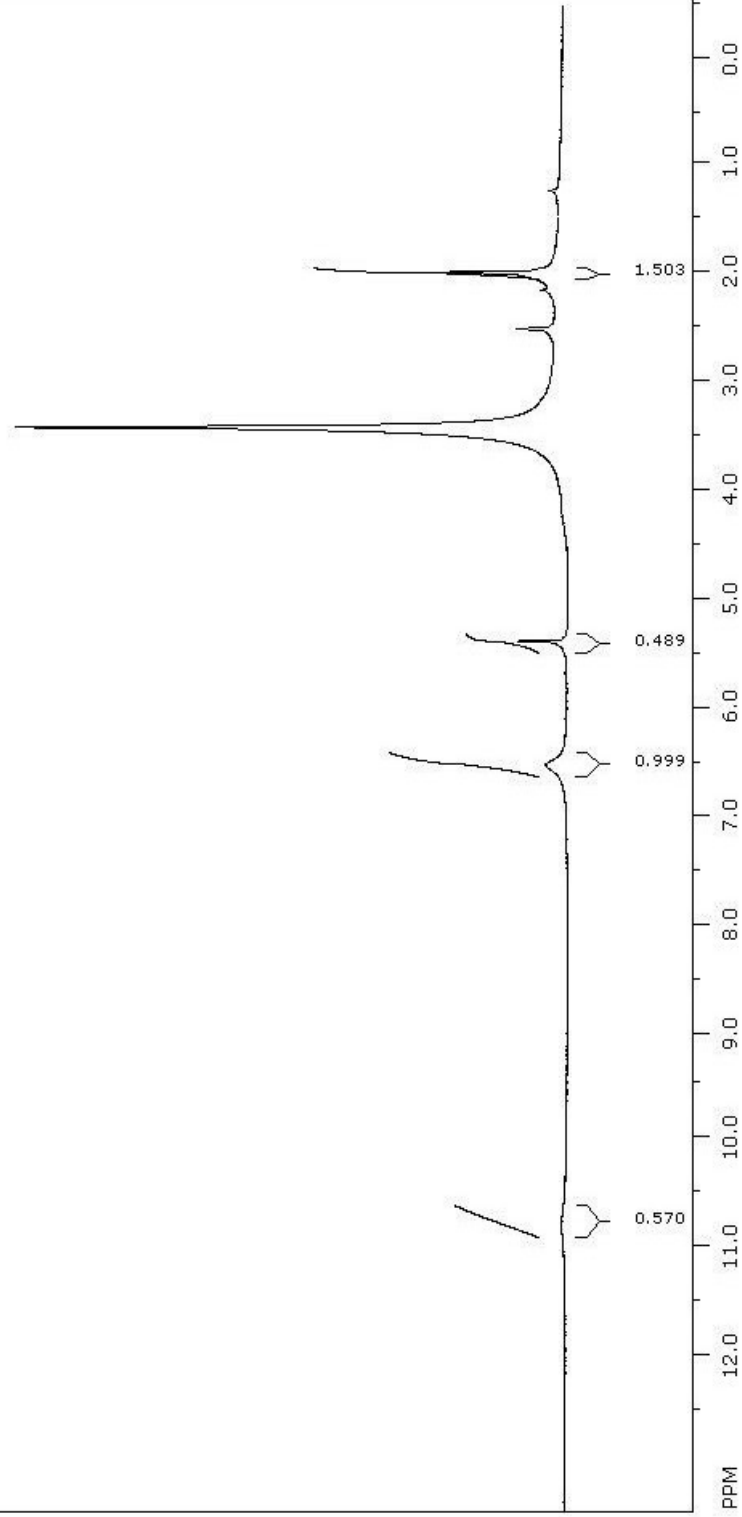
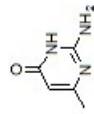
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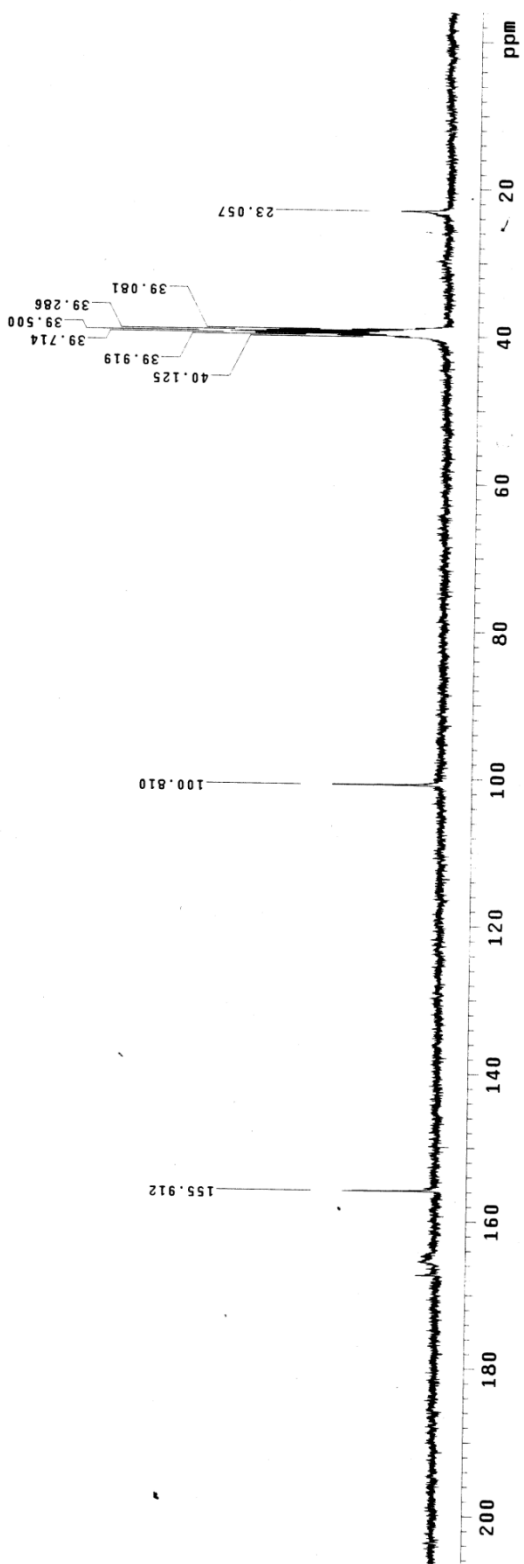


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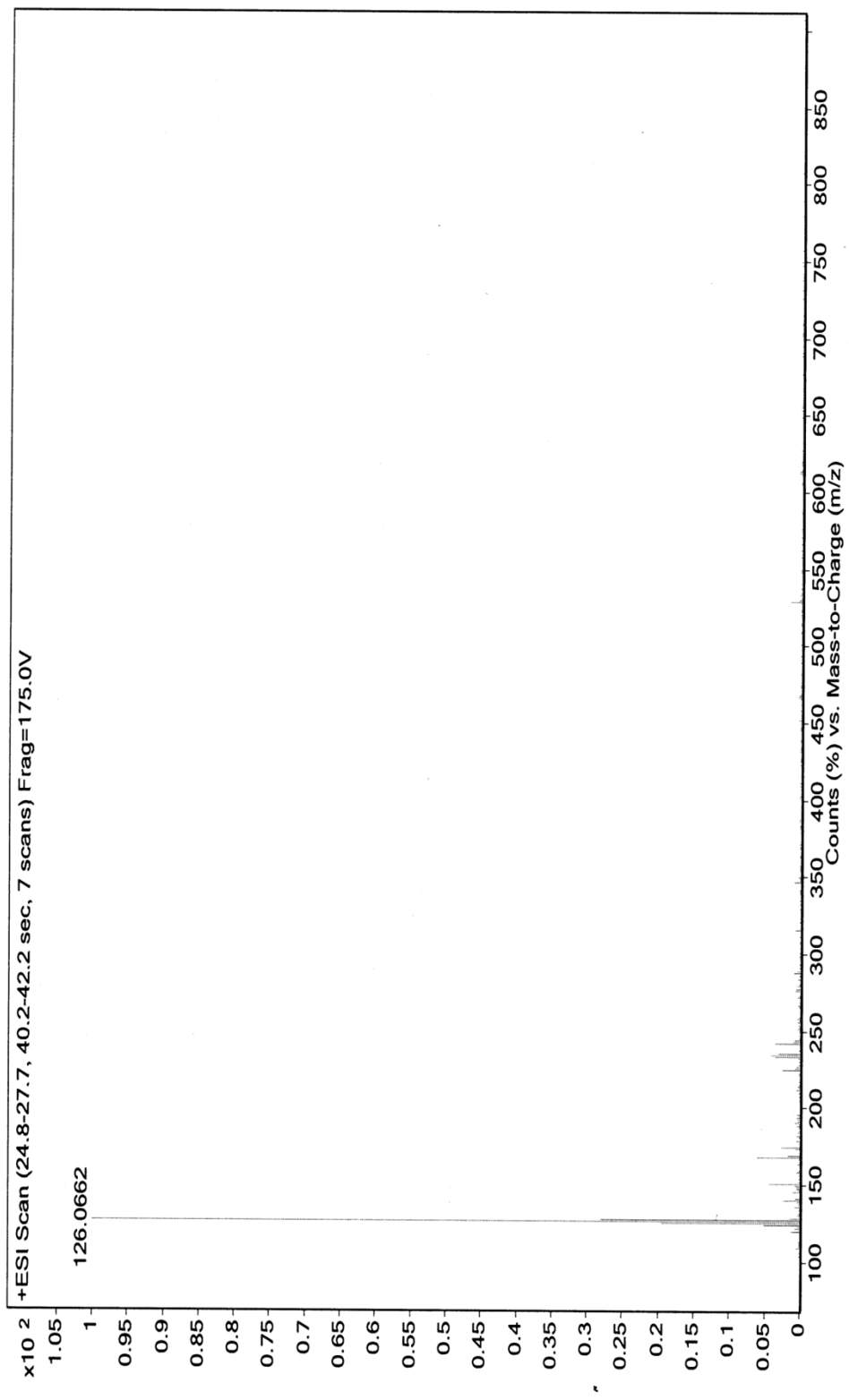


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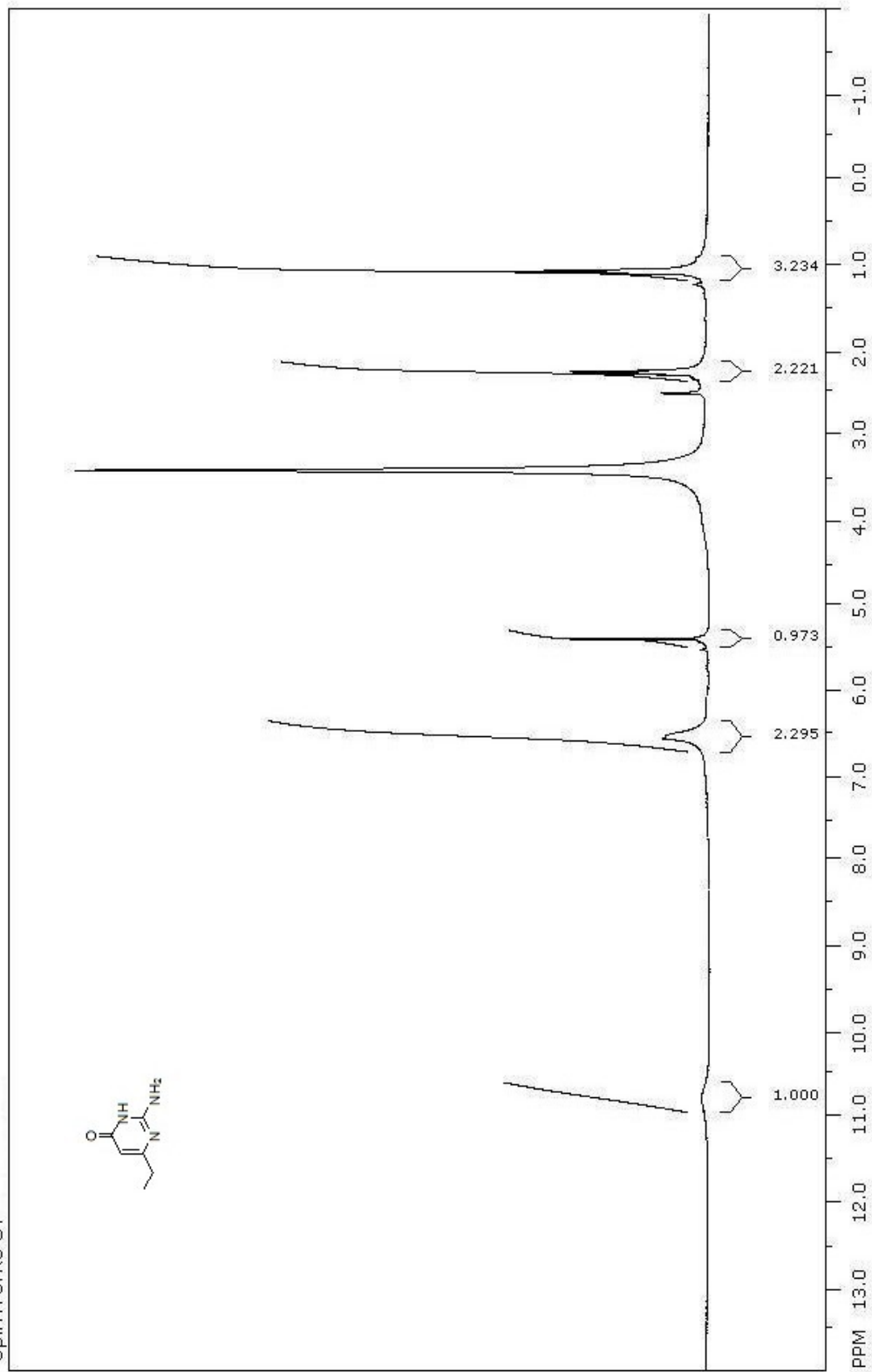
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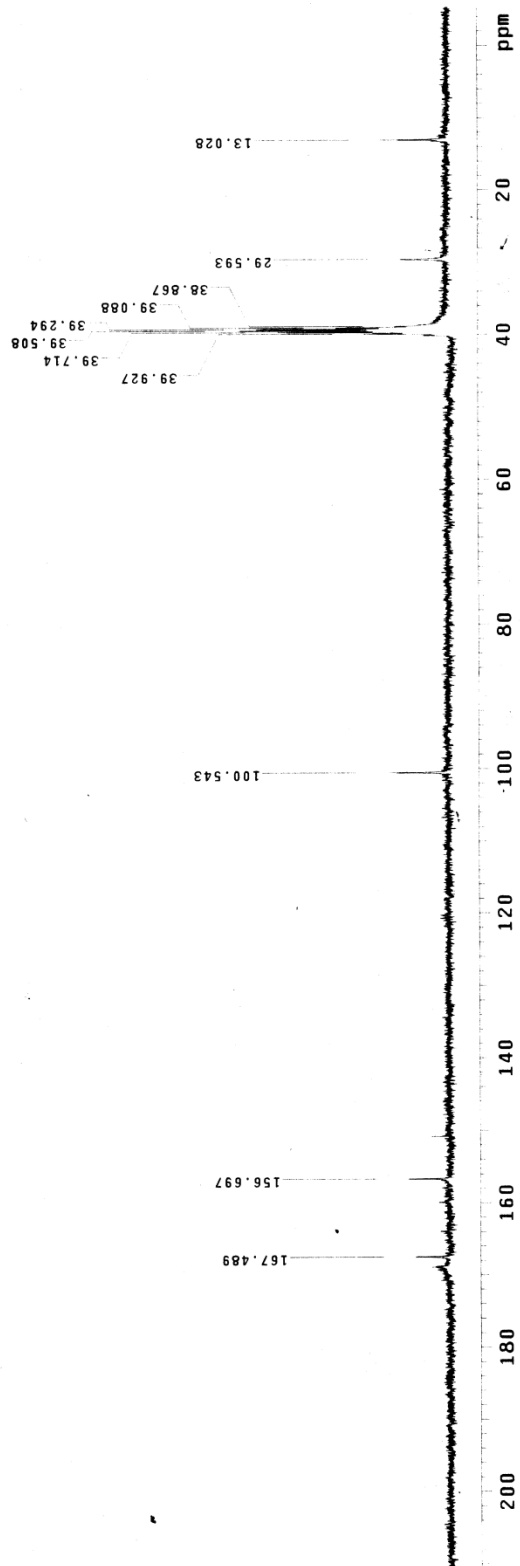
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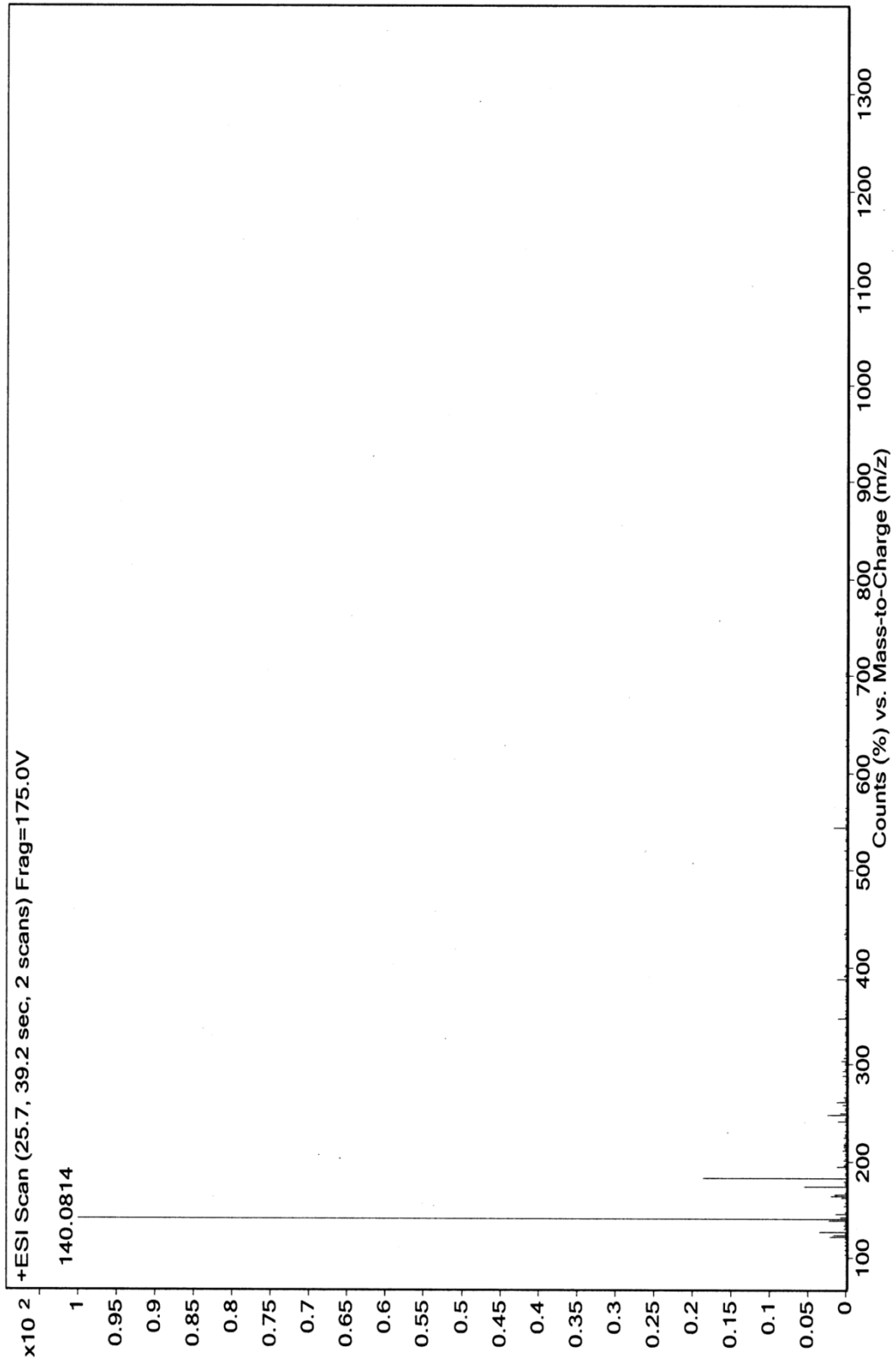


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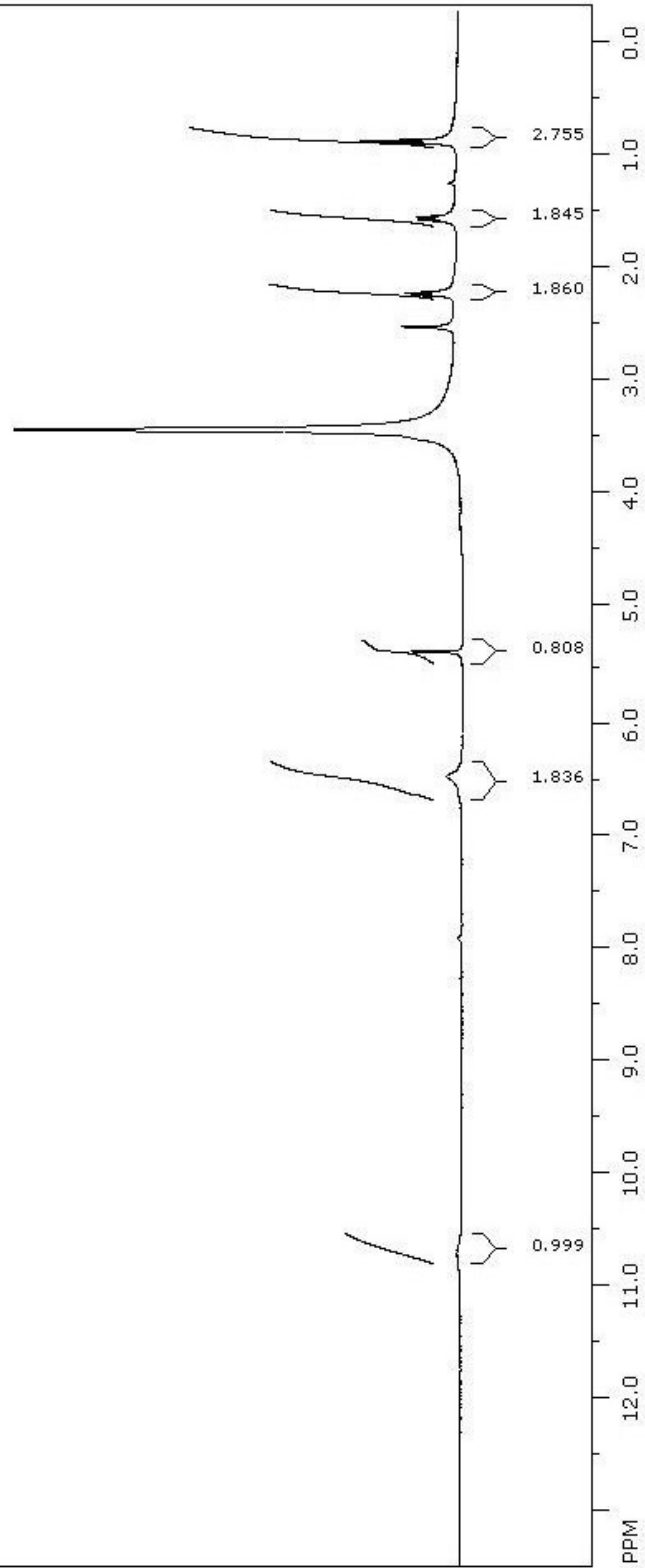
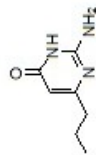
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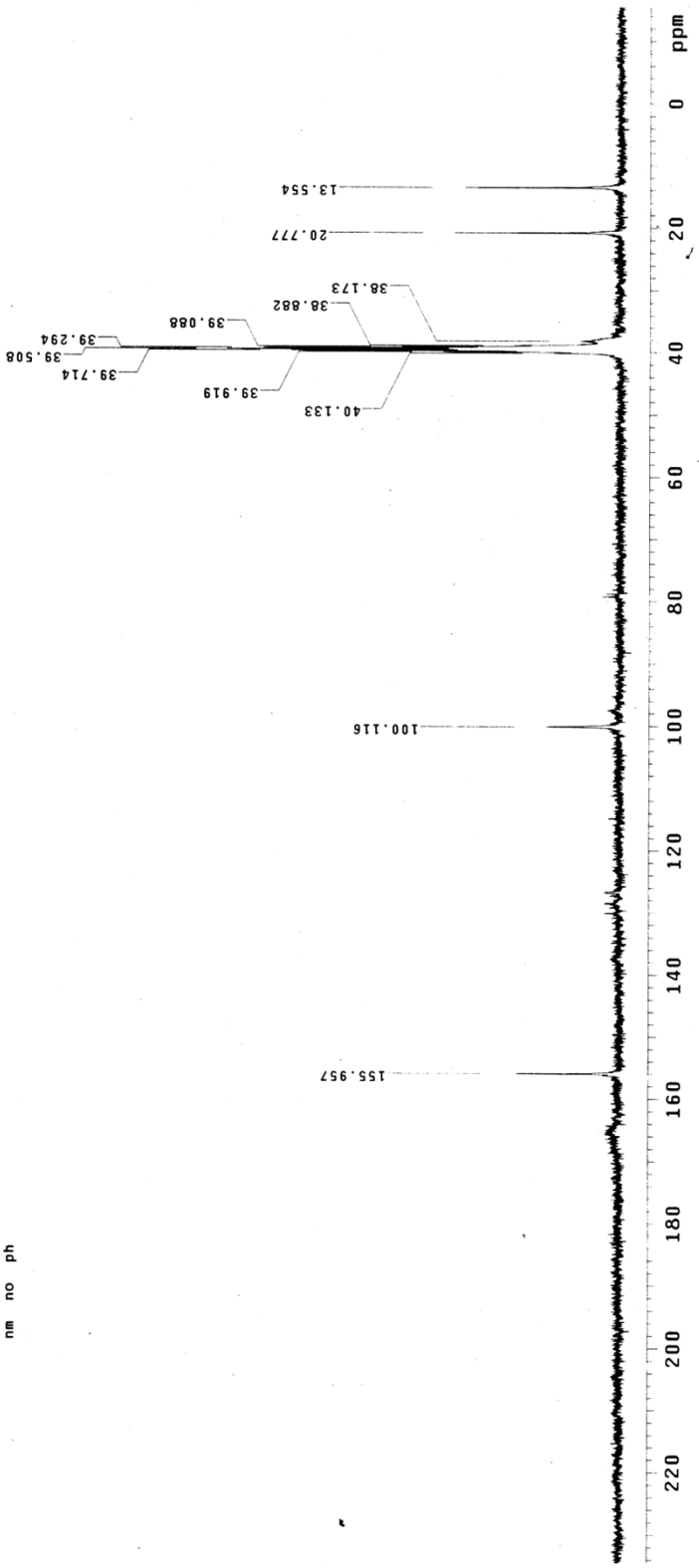


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 dpr 8900 th 62  
 dmf nm no ph 4



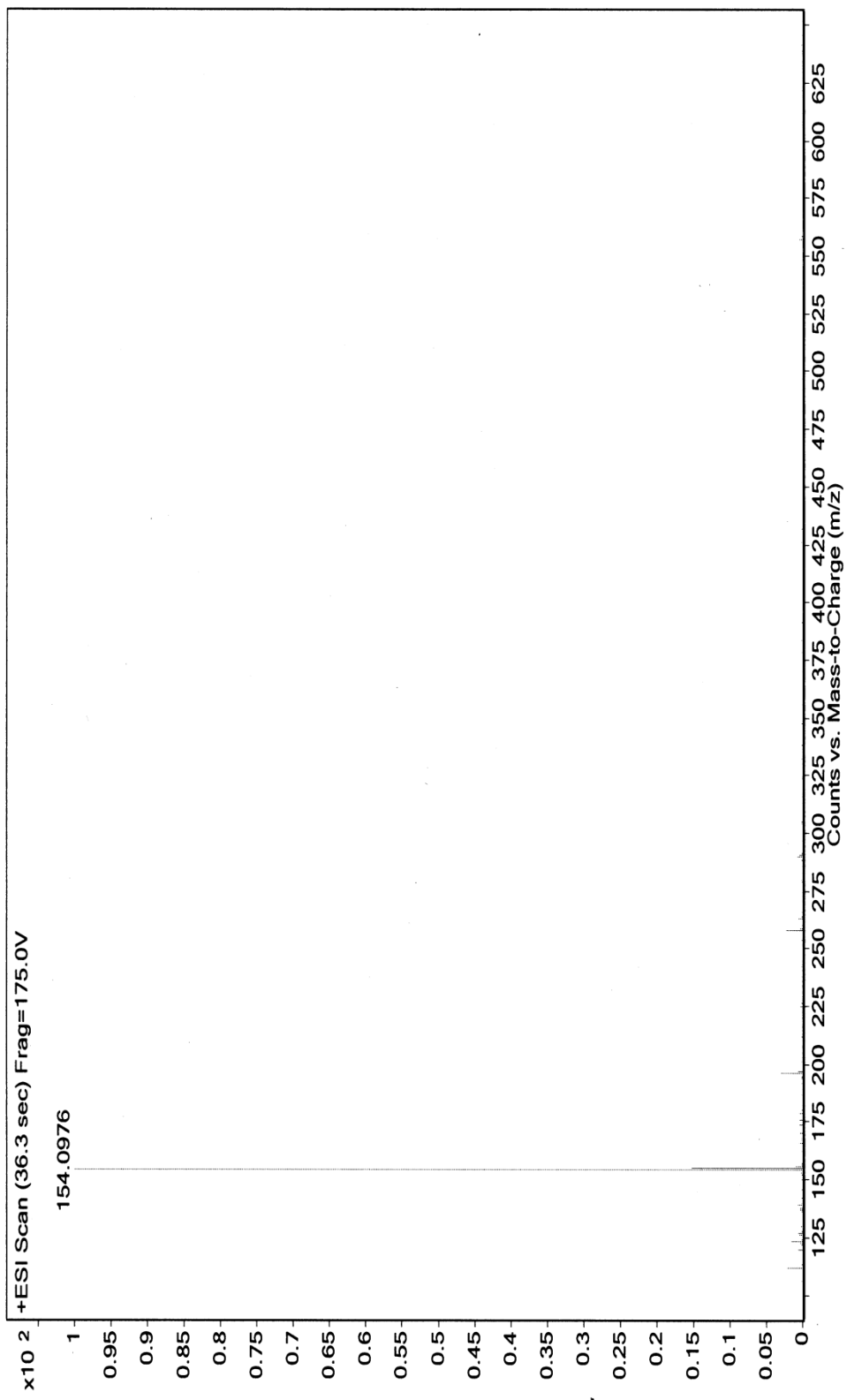


Sample Name  
Inj Vol  
Data Filename

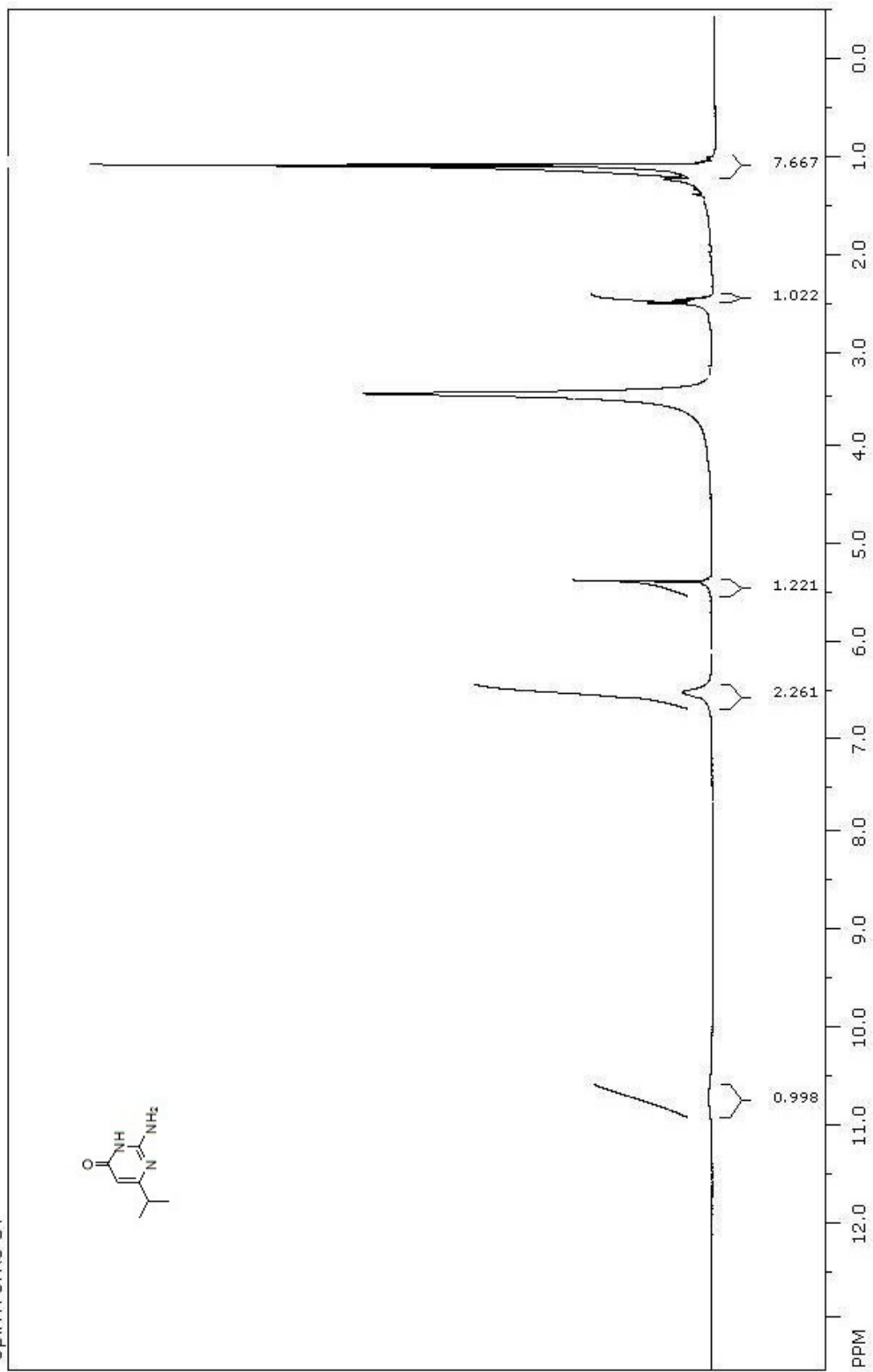
Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time



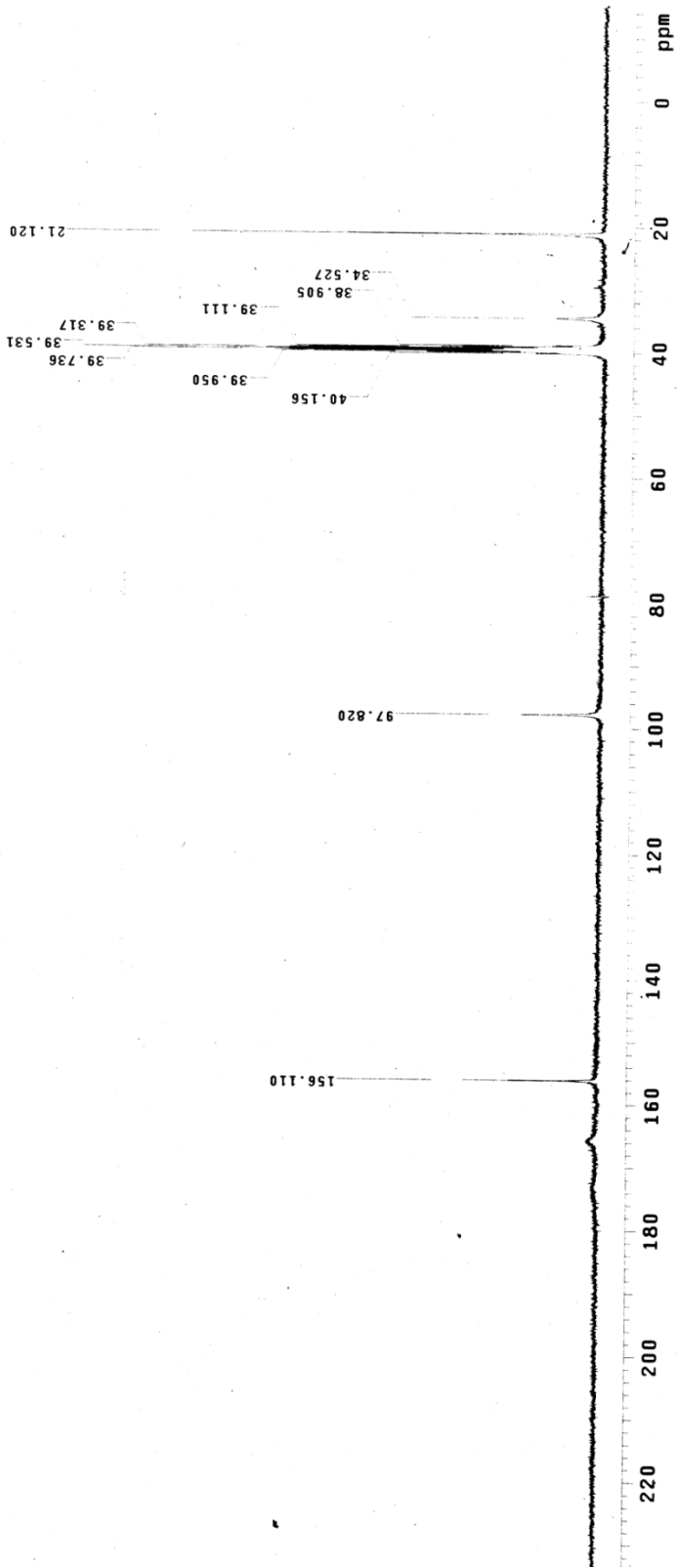
SpinWorks 3:



file: ...shnan\NMR-DATE\KTK-GUA-ISO.fid\fid block# 1 expt: "s2pul"  
transmitter freq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32  
freq. of 0 ppm: 399.852856 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 224.811 ppm/cm: 0.56223

SAMPLE SPECIAL

date	Jun 30 2012	temp	not used
solvent	DMSO	gain	not used
file	exp	sp1n	not used
sw	ACQUISITION	hst	0.008
at	25125.6	pw90	18.600
np	1.199	alfa	20.000
td	6270	ll	FLAGS
ds	13800	ll	n
nt	1.20	ln	n
ct	1.000	dp	y
	1.000	hs	PROCESSING
	1520	ns	nn
tn	TRANSMITTER	lb	2.00
sfrq	C13	fn	65536
tof	100.554	sp	DISPLAY
tpwr	1536.3	wd	-1547.2
	61	rf1	25125.6
	9.300	rf2	5518.6
dn	DECOUPLER	rp	3971.5
dof	H1	lp	-21.8
dm	0	pl	-351.5
dmm	yyy	wc	PLOT
dpwr	42	sc	250
dat	8900	vs	0
		th	66
		nm	66
		no	5
		ph	

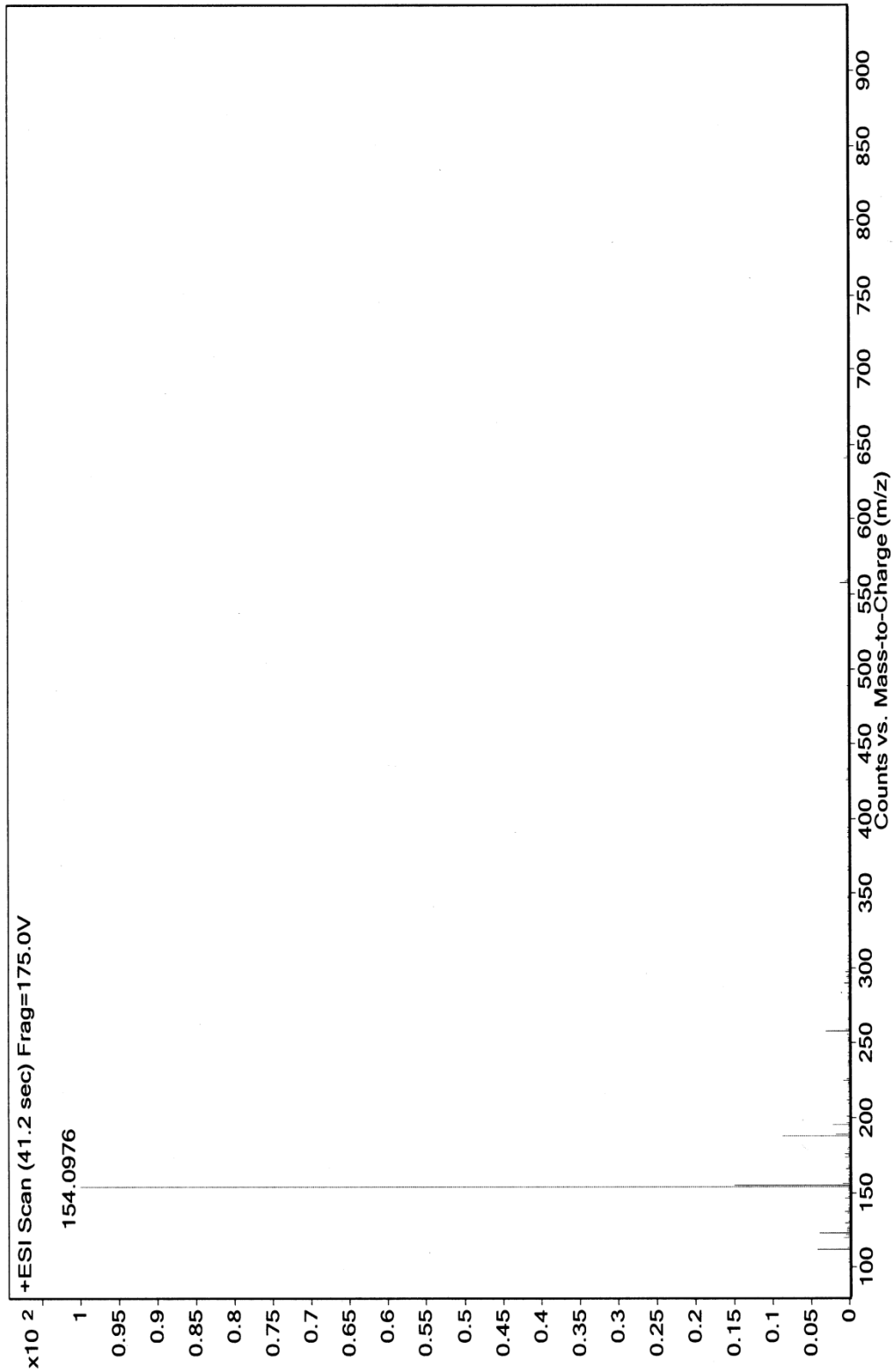


Sample Name  
Inj Vol  
Data Filename

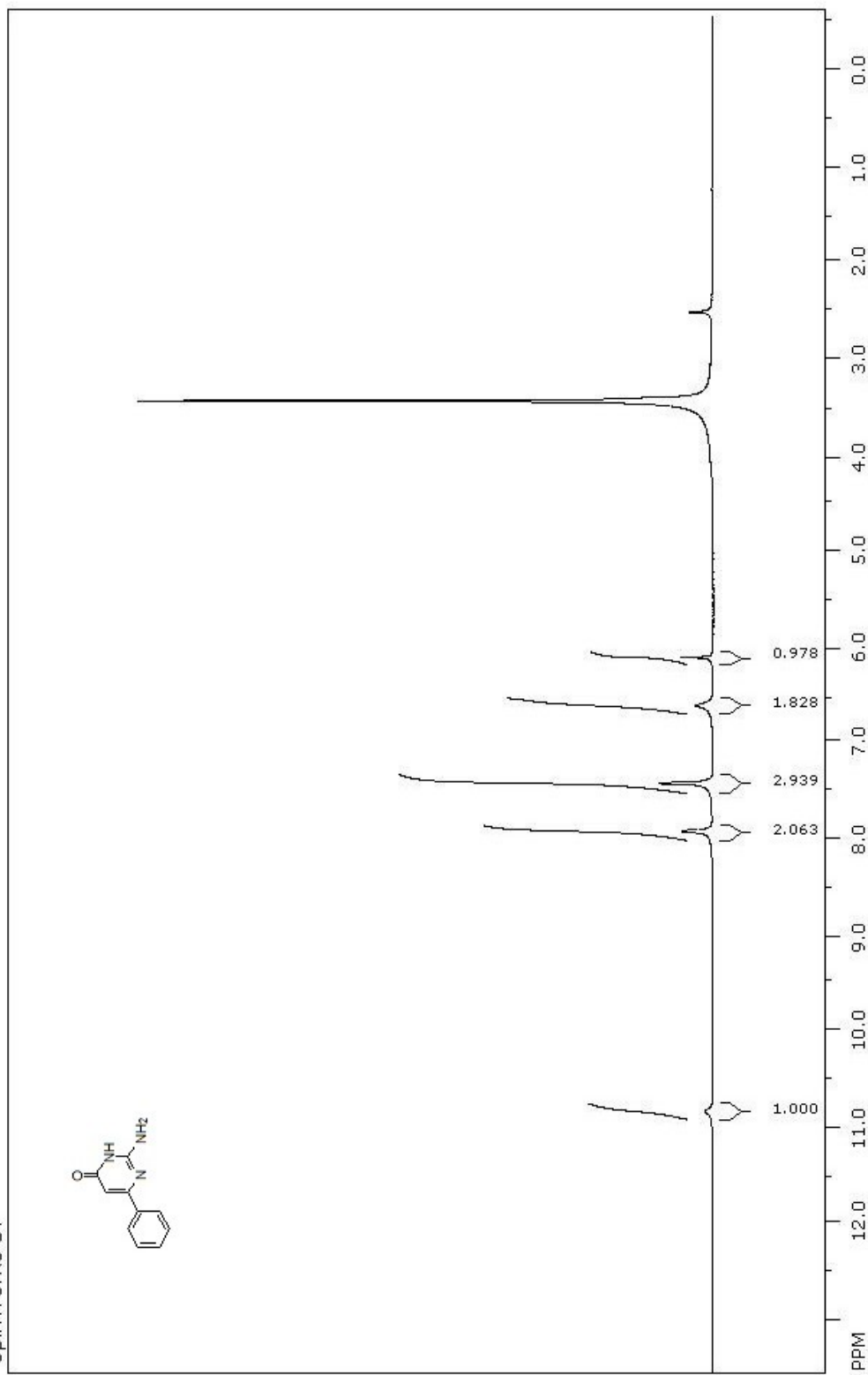
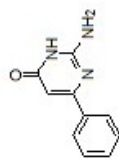
Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time

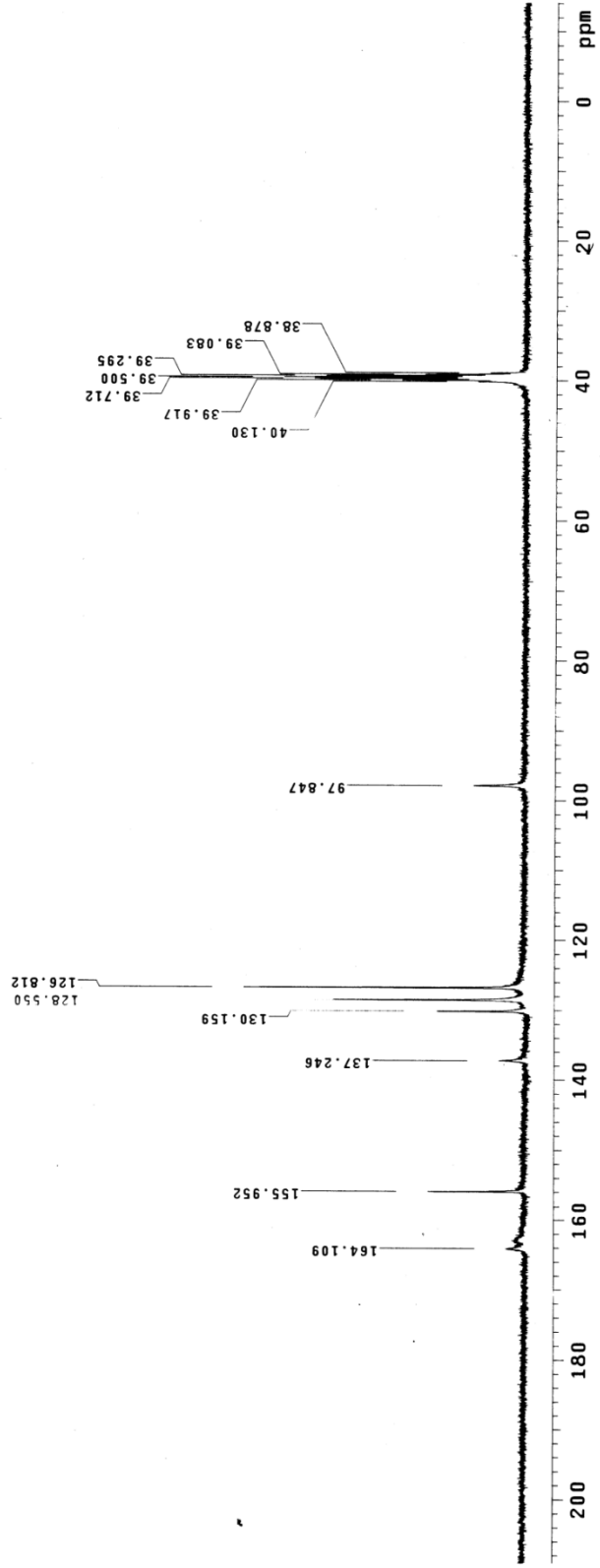


SpinWorks 3:



file: ...ishnan\NMR-DATA\KRR-PH-GUA.fid\fid block# 1 expt: "s2pul"  
transmitter freq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32  
freq. of 0 ppm: 399.852855 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 227.149 ppm/cm: 0.56808

SAMPLE date Jul 5 2012 SPECIAL temp not used  
 solvent DMSO gain not used  
 file ACQUISITION exp not used  
 sw 25000.0 hsc not used  
 at 1.199 dTf 18.006  
 np 59968 dTfA 20.000  
 bs 13800 fl n  
 d1 0 dp n  
 nt 5000' hs n  
 ct 3360 PROCESSING nn  
 tn TRANSMITTER lb 1.00  
 sfrq 100.553 fn not used  
 tof 0 sp -1419.6  
 tpr 61 wp 22437.2  
 pw 8.667 rfl 7000.2  
 dn DECOUPLER H1 rfp 3971.5  
 dof 0 lp -29.5  
 dm vvy wc PLOT -393.6  
 dmm 250  
 dpr 42  
 dnr 8900  
 dnt 44  
 nm no ph 2

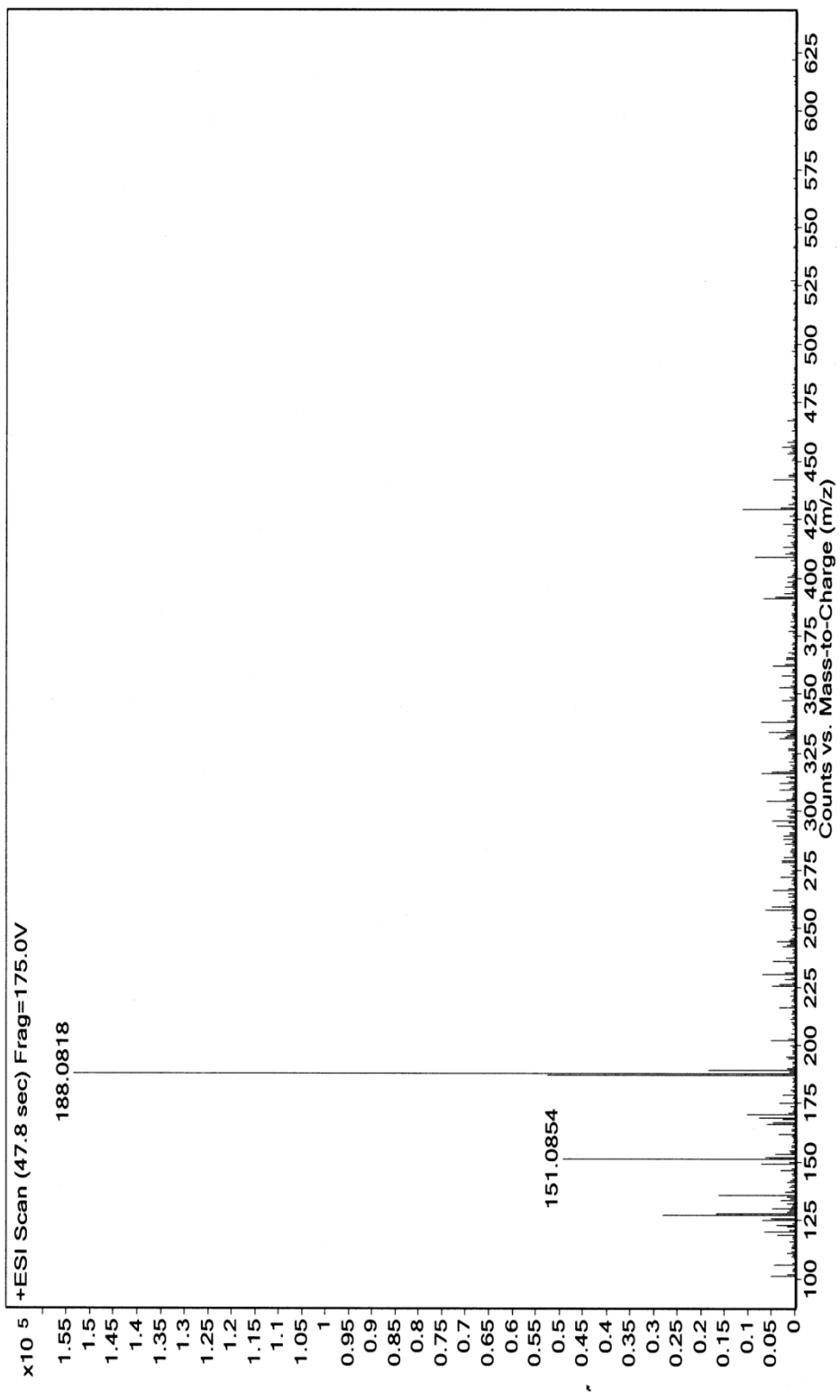


User Name  
IRM Calibration Status  
Acquired Time

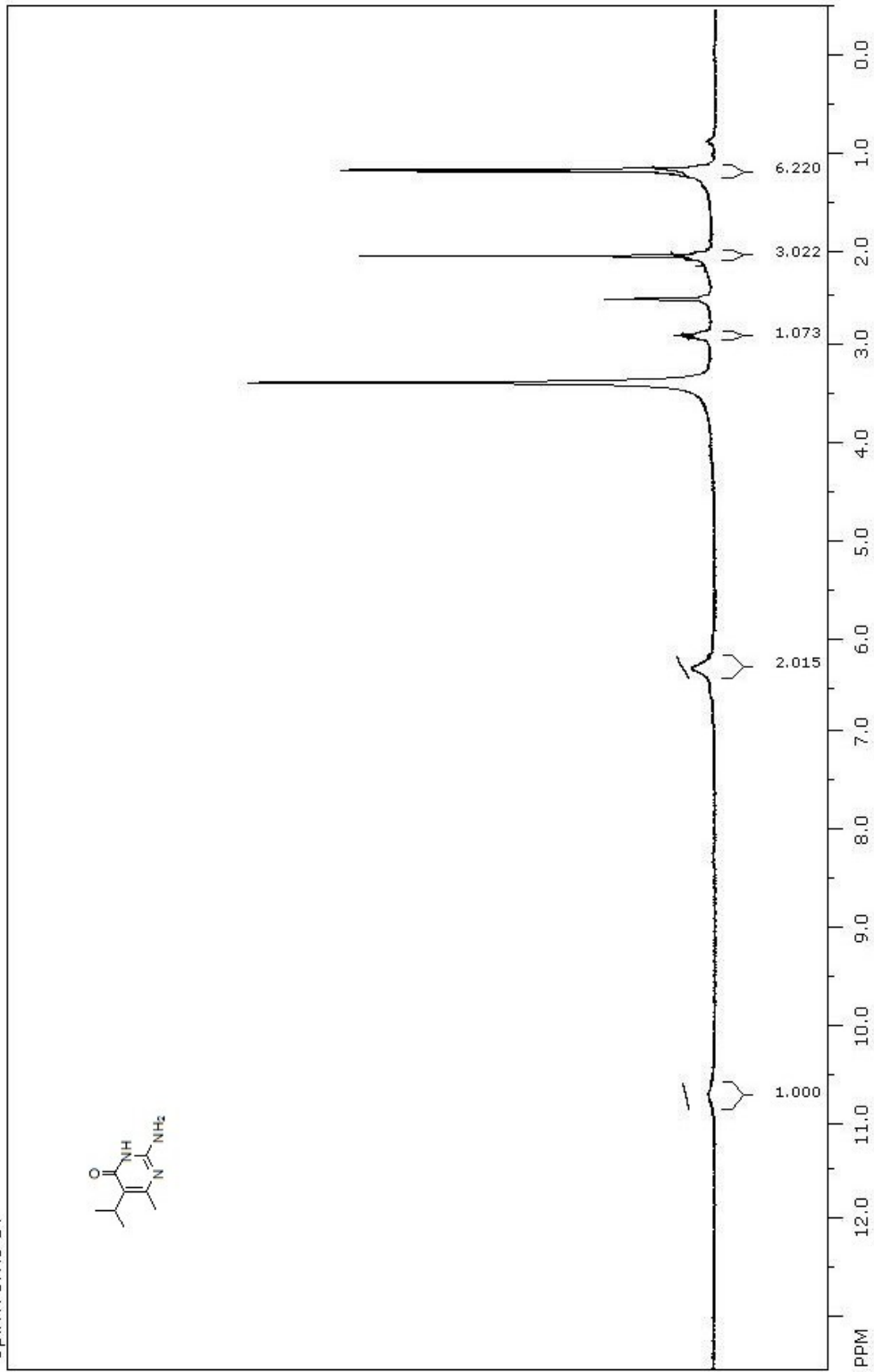
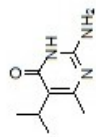
Instrument Name  
SampleType  
Comment

Position  
InjPosition  
ACQ Method

Sample Name  
Inj Vol  
Data Filename



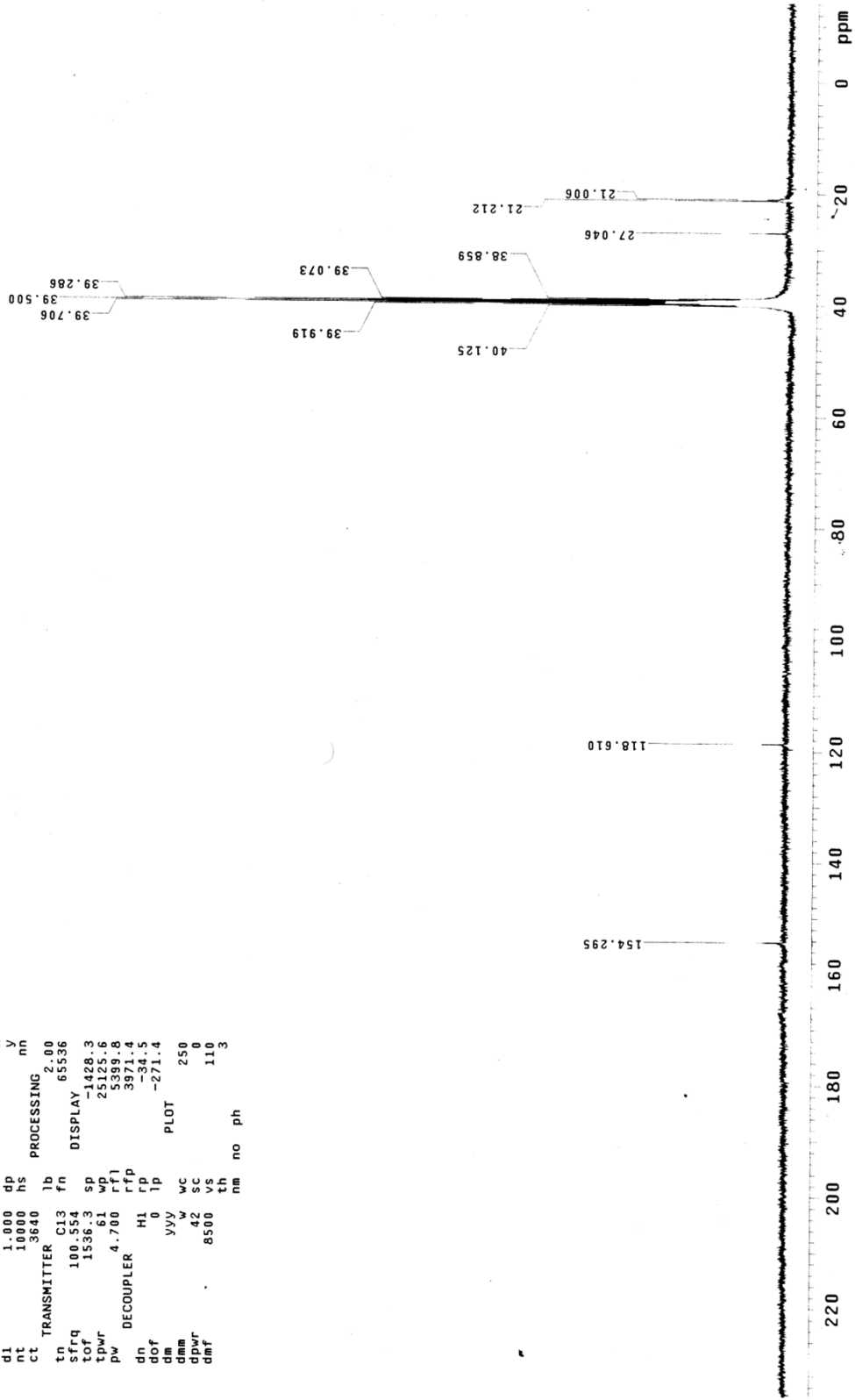
SpinWorks 3:



file: ...an\NMR-DATA\KRK-GUA-ME-ISO.fid\fid block # 1 expt: 's2pul'  
transmitterfreq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 2  
freq. of 0 ppm: 399.852853 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 225.006 ppm/cm: 0.56272



SAMPLE May 12 2013 temp not used  
 solvent DMSO gain not used  
 FILE ACQUISITION exp spin not used  
 hst 0.008  
 pw90 3.400  
 at 25125.6  
 60270 alfa 20.000  
 np 13800 il FLAGS  
 fb 13800 il n  
 bs 1.000 dp n  
 dl 10000 hs V  
 nt 10000 hs  
 ct 3640 PROCESSING nn  
 tn TRANSMITTER lb 2.00  
 C13 fn 65536  
 sfrq 100.554 DISPLAY  
 tof 1536.3 sp -1428.3  
 tpwr 61 wp 25125.6  
 pw 4.700 rfl 5389.8  
 DECOUPLER H1 rfp 3971.4  
 dn 0 rp -34.5  
 dot 0 lp PLOT -271.4  
 dm vvy w wc 250  
 dmm w 42 SC 0  
 dpwr 8500 VS 110  
 dnr nm no ph 3

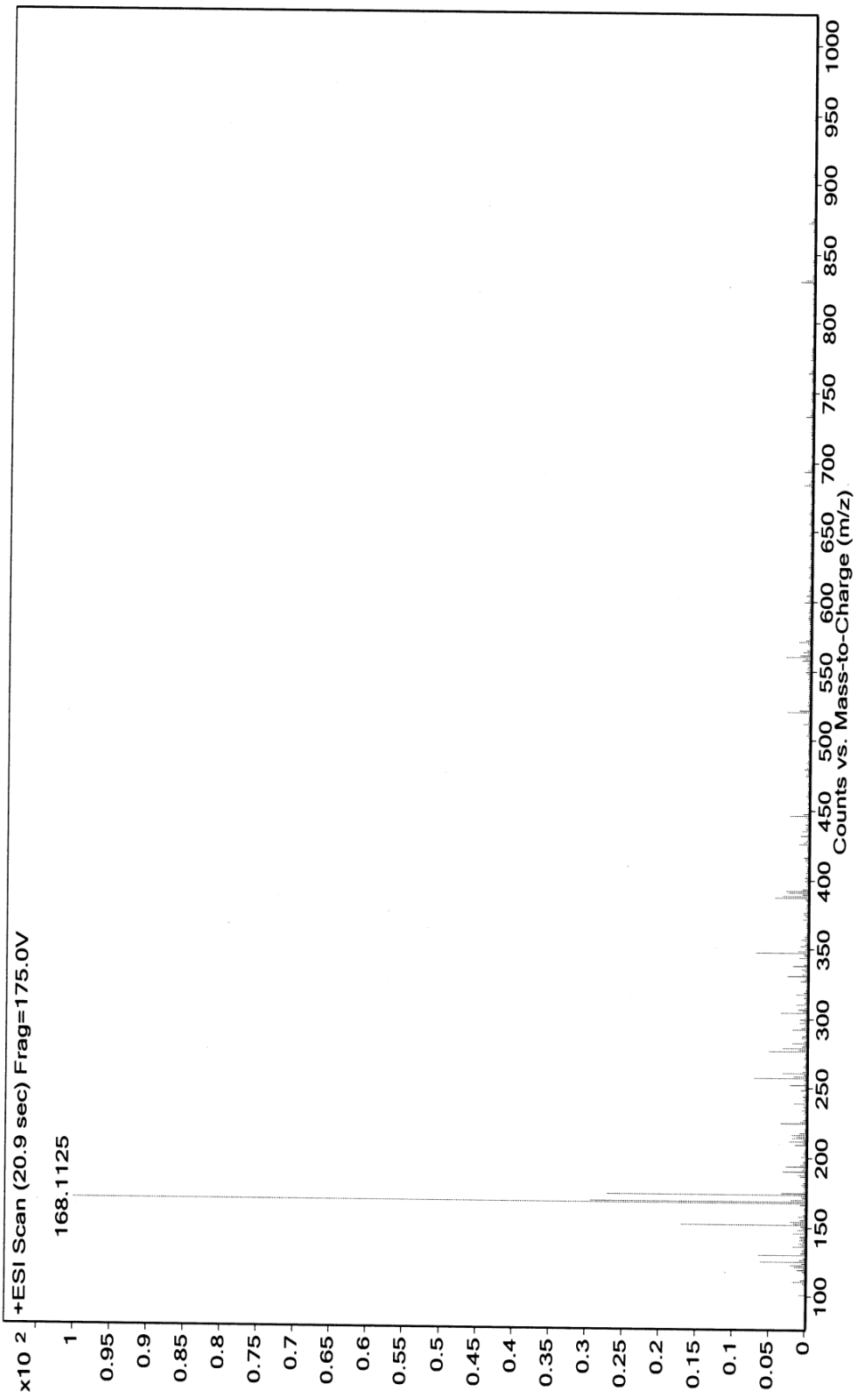


Sample Name  
Inj Vol  
Data Filename

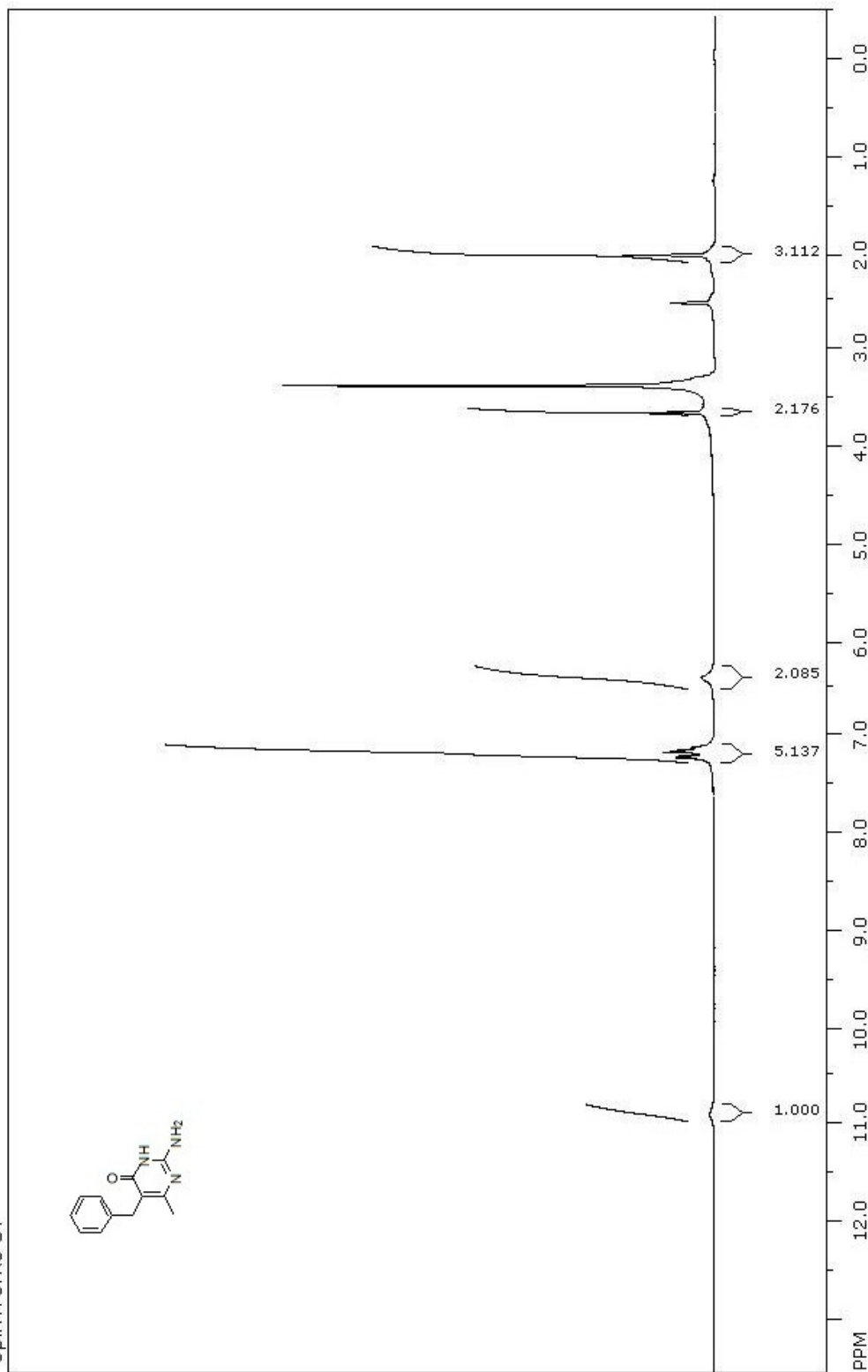
Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time



SpinWorks 3:



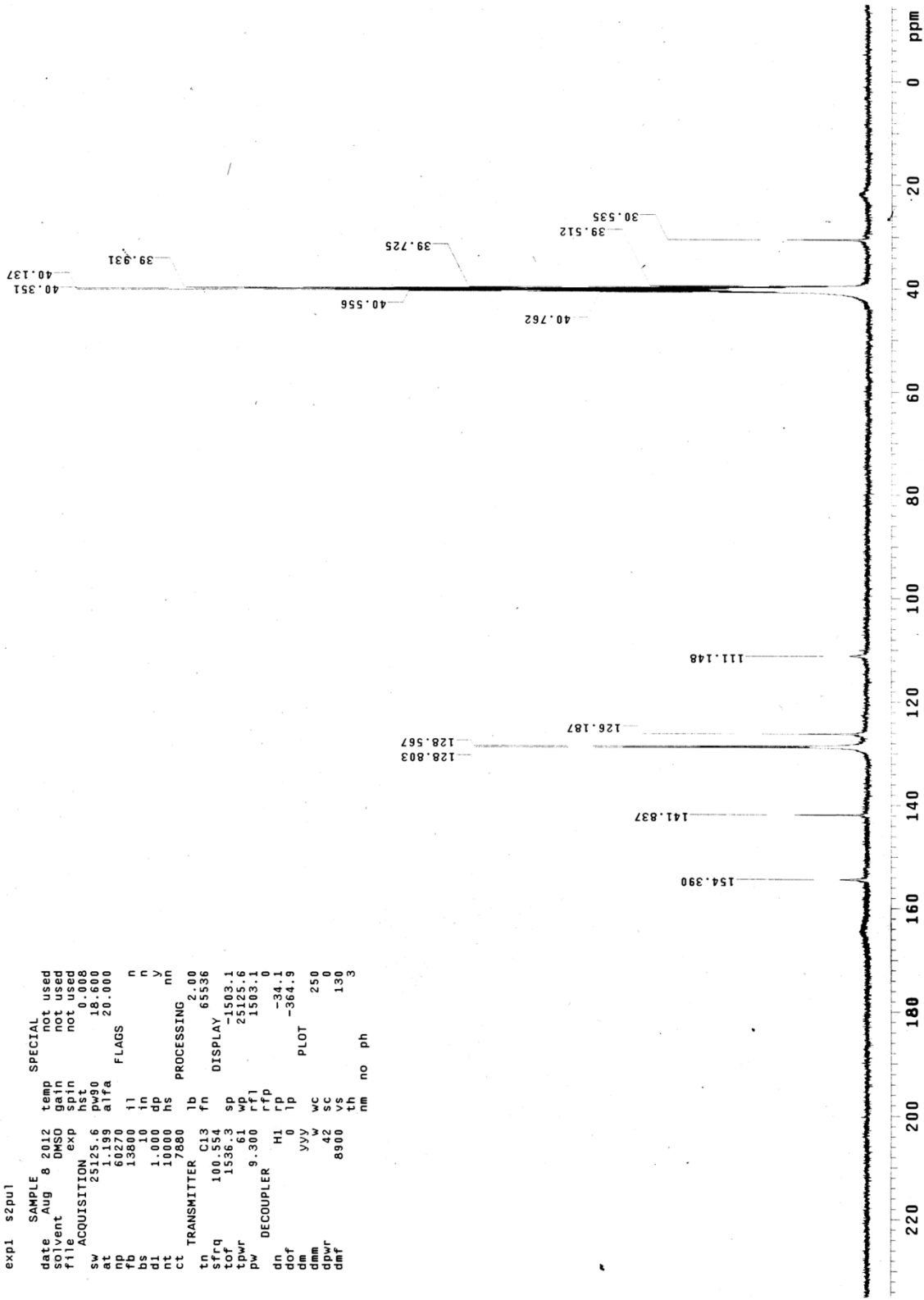
file: ...nan\NMR-DATA\KRR-GUA-ME-BZ.fid\fid block# 1 expt: "s2pul"  
transmitter freq.: 399.85262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32

freq. of 0 ppm: 399.852856 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 225.395 ppm/cm: 0.56369

KRK-MBZ-1-13C

expl szpu1

SAMPLE SPECIAL  
date Aug 8 2012 temp not used  
solvent DMSO gain not used  
flievent exp not used  
sp in not used  
sw ACQUISITION 25125.6 hs 0.00  
at 11199 p90 18.00  
np 60270 atfa 20.000  
fb 13800 ll  
bs 10 in u  
di 1.000 dp y  
nt 10000 hs  
ct 7880  
TRANSMITTER lb 2.00  
tn C13 fn 65536  
sfrq 100.554  
tof 1536.3 sp -1503.1  
tpwr 61 wp 25125.6  
pw 9.300 rfl 1305.1  
DECOUPLER H1 rfp -34.1  
dn 0 lp -364.9  
dof vvv wc 250  
dm w sc 42  
dmm vs 130  
dpwr 8900  
dmf th no ph 3

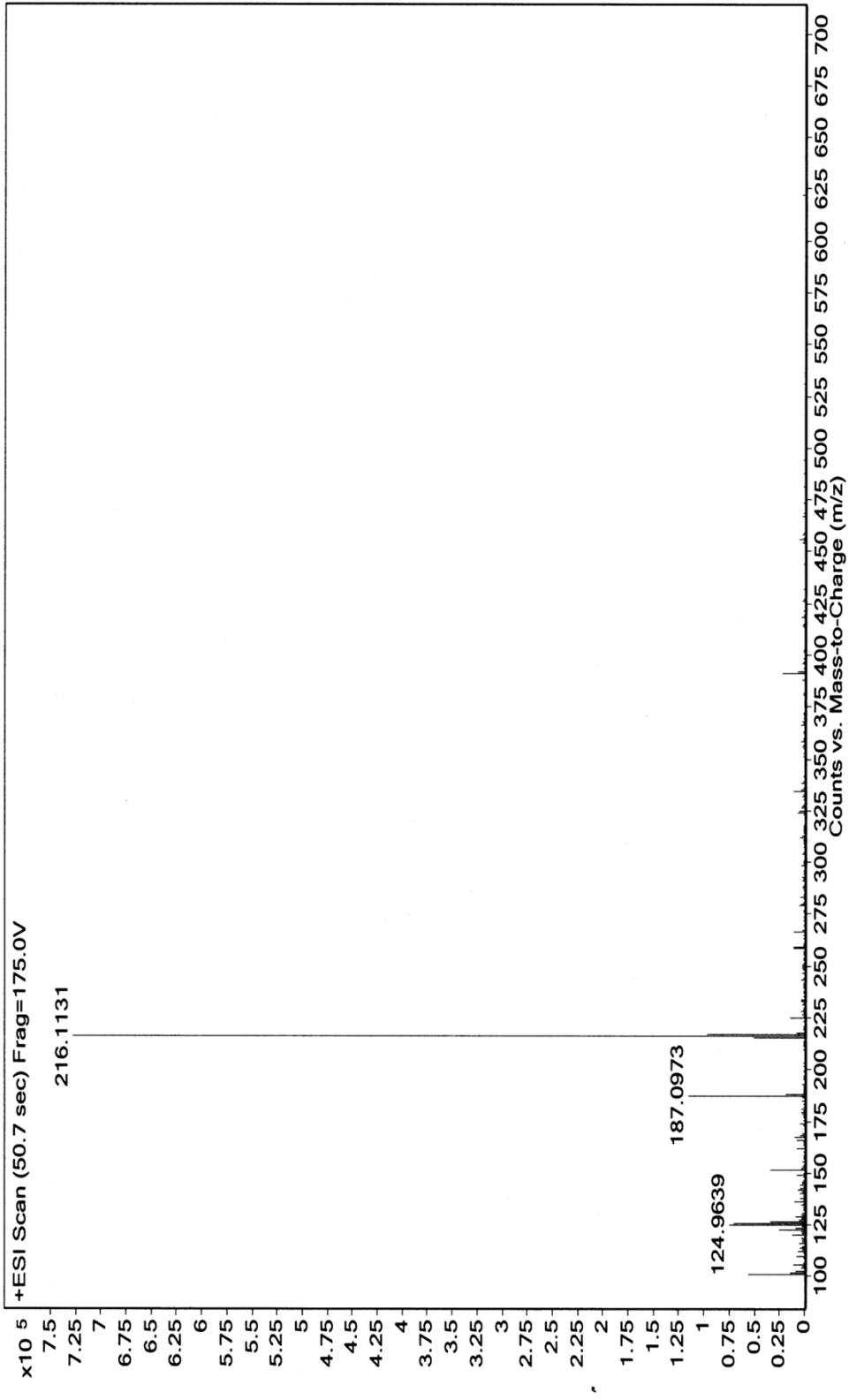


Sample Name  
Inj Vol  
Data Filename

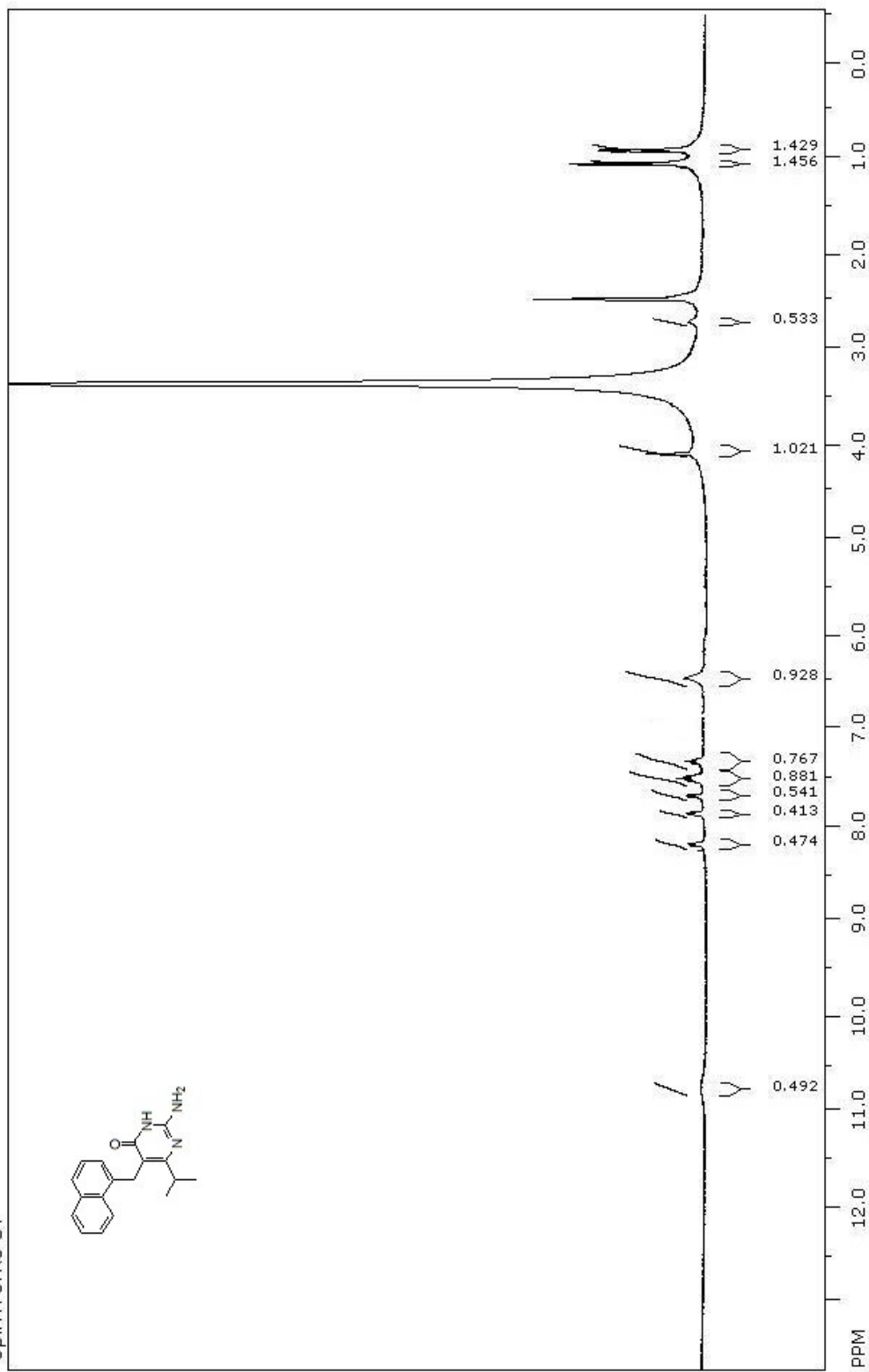
Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time

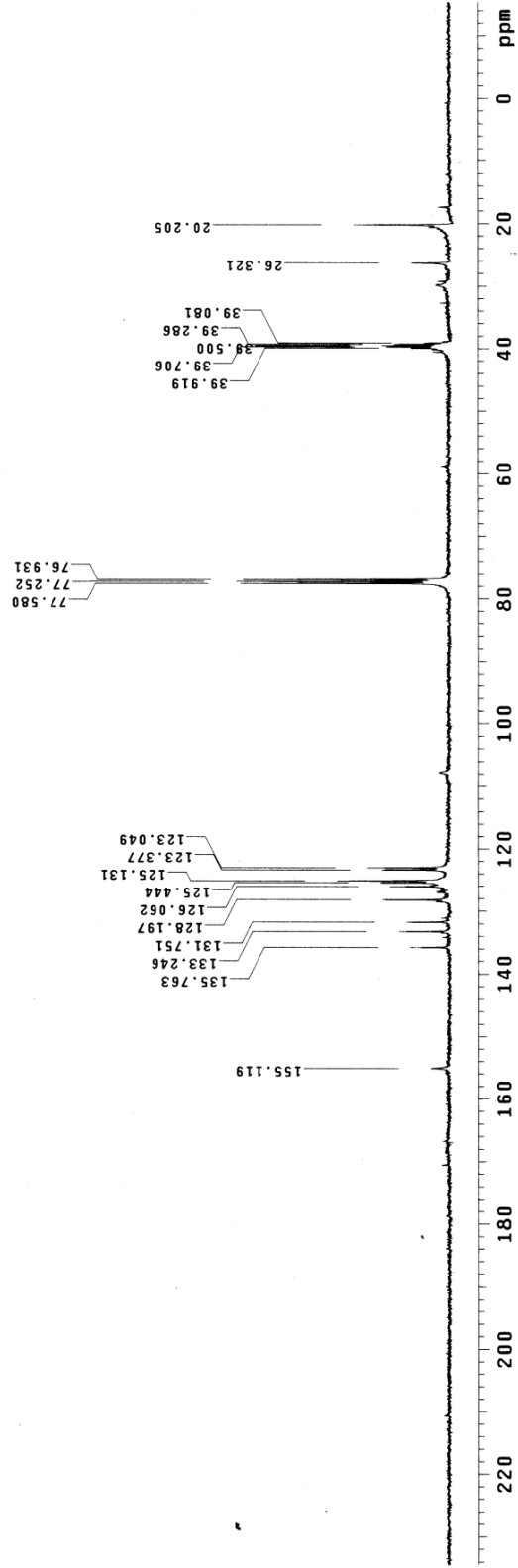


SpinWorks 3:



file: ...an\NMR-DATA\KRK-ISO-NAPH-H.fid\fid block# 1 expt: "s2pul"  
transmitter freq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32  
freq. of 0 ppm: 399.852863 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 228.123 ppm/cm: 0.57051

SAMPLE SPECIAL  
 date Sep 26 2012 temp not used  
 solvent CDCl3 gain not used  
 file /export/home/~ spin not used  
 appel/KRK-ISO-MAPH-hst 0.008  
 -13C.fid pw90 18.600  
 alfa 20.000  
 SW ACQUISITION FLAGS  
 at 25125.6 il n  
 fp 64270 in v  
 bp 13800 dp v  
 bs 110 hs nm  
 d1 1.000 lb 2.00  
 nt 15000 fn 65536  
 ct TRANSMITTER C13 sp -1550.3  
 tn 100.554 wp 25125.6  
 sfrq 1536.3 rfl 5521.7  
 tpwr 61 rfp 3971.4  
 pw 9.300 rp -14.3  
 DECOUPLER H1 lp -397.2  
 dn HI PLOT  
 dof 0 wc 250  
 dm yy sc 0  
 dmm w vs 33  
 dpwr 42 th no ph  
 dmf 8900 nm no ph

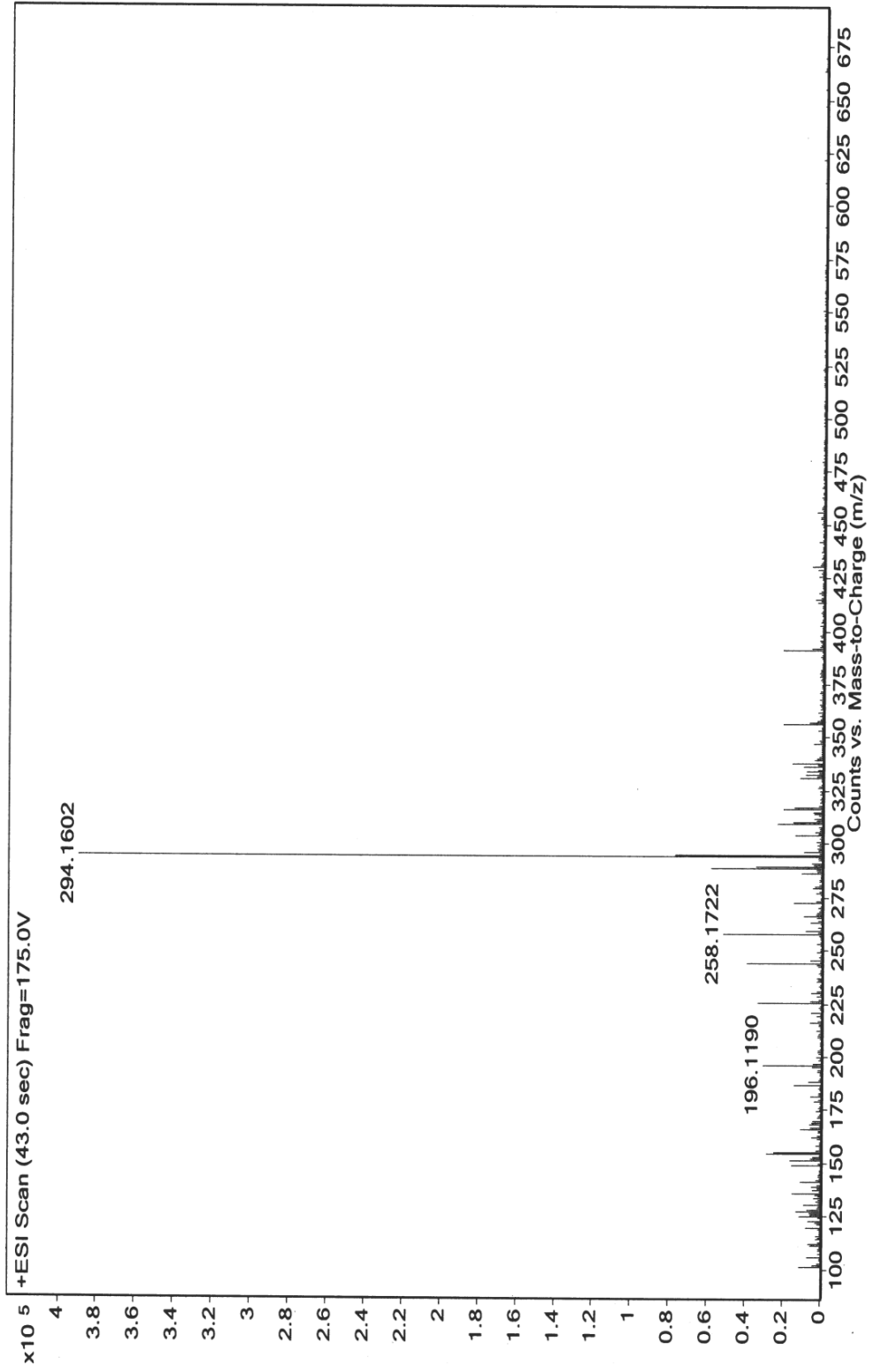


Sample Name  
Inj Vol  
Data Filename

Position  
InjPosition  
ACQ Method

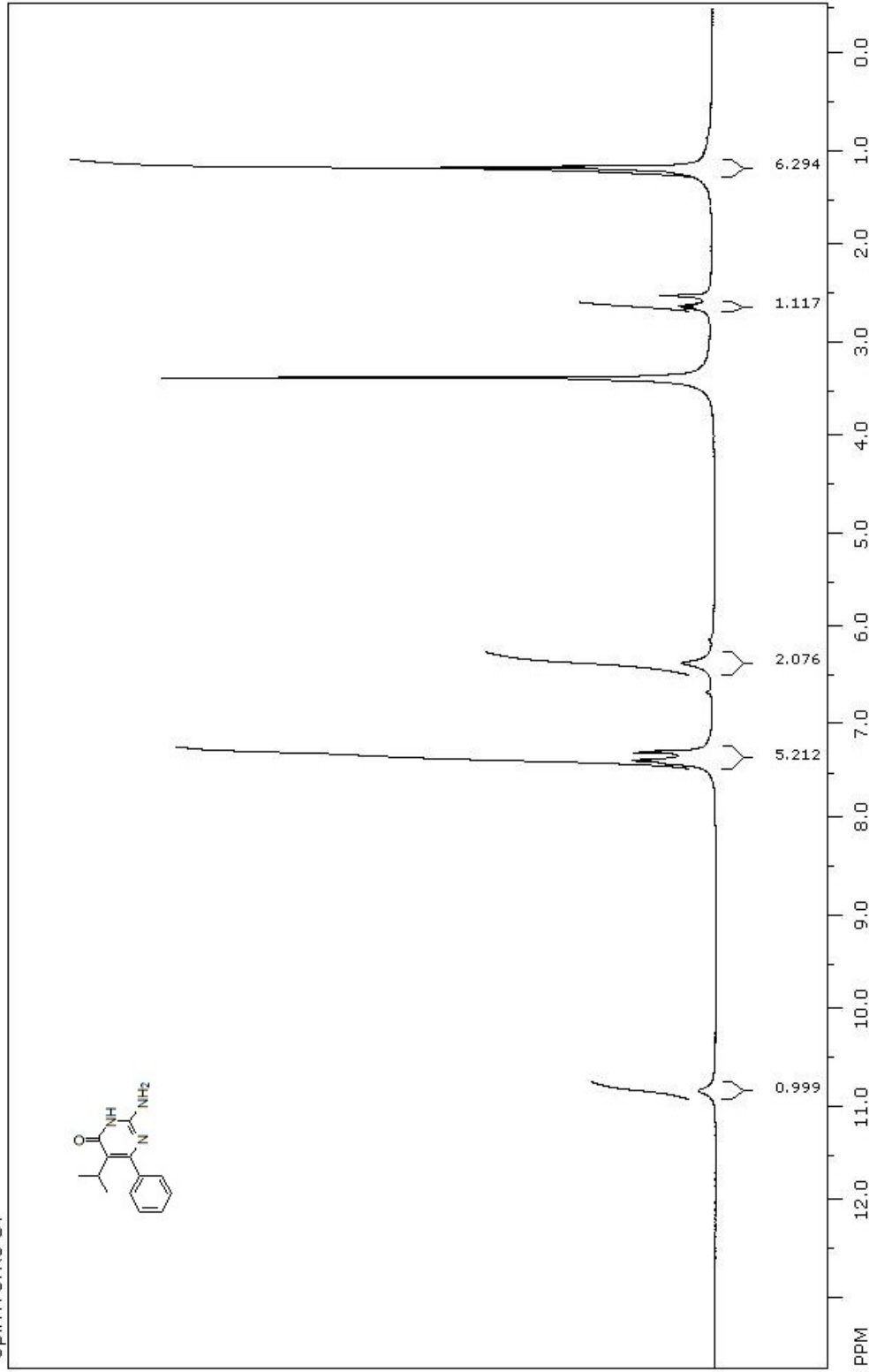
Instrument Name  
Sample Type  
Comment

User Name  
IRM Calibration Status  
Acquired Time



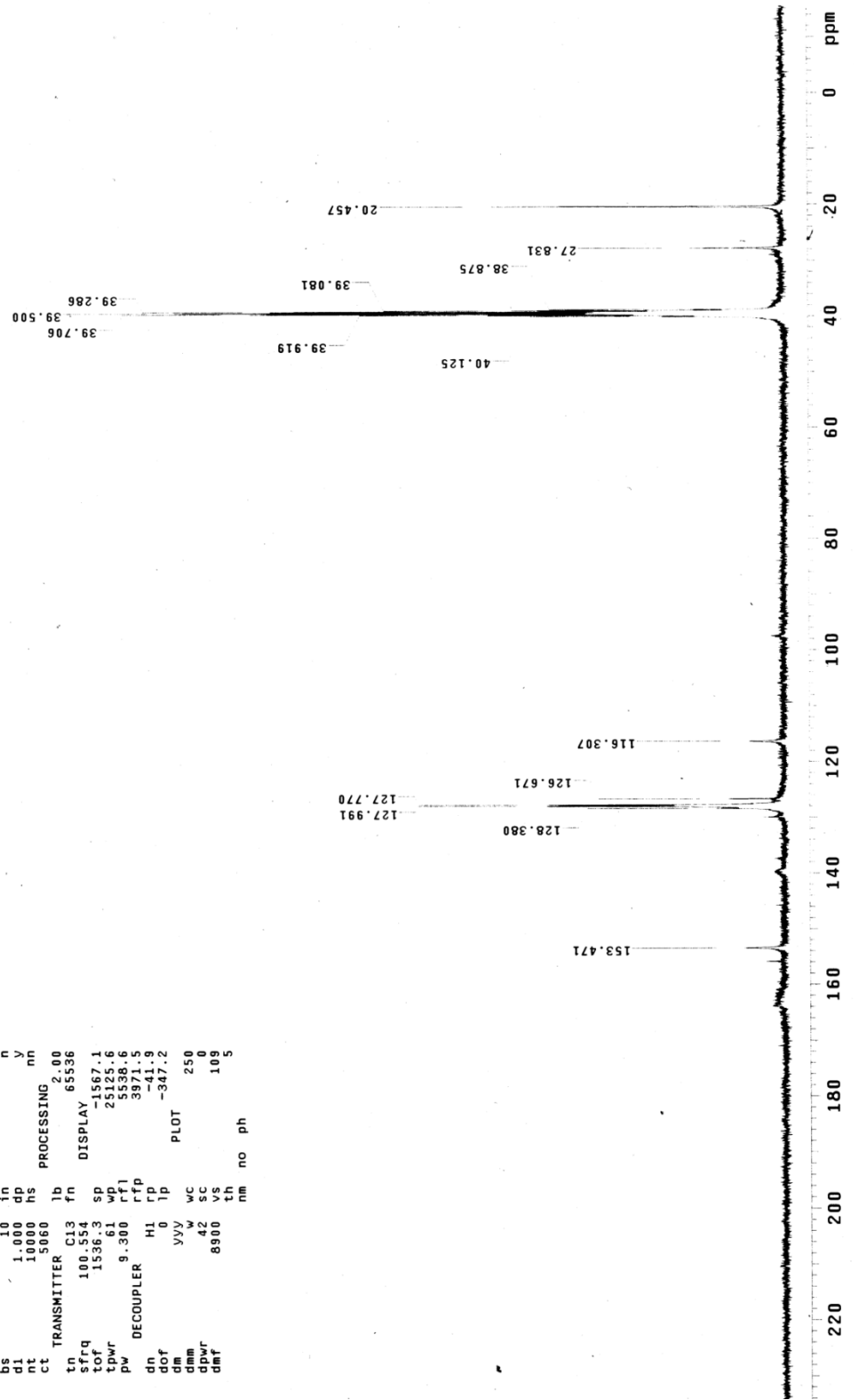


SpinWorks 3:



file: ...an\NMR-DATA\KRK-GUA-PH-ISO.fid\fid block# 1 expt: "s2pul"  
transmitter freq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32  
freq. of 0 ppm: 399.852857 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 228.512 ppm/cm: 0.57149

SAMPLE SPECIAL  
 date Aug 30 2012 temp not used  
 solvent DMSO gain not used  
 file exp not used  
 ACQUISITION hst 0.008  
 sw 25125.6 pw90 18.600  
 at 1.199 alfa 20.000  
 np 60270 ll  
 fb 13800 ll n  
 bs 10 ln n  
 dl 1.000 dp y  
 nt 15000 hs nm  
 ct TRANSMITTER C13 lb PROCESSING 2.00  
 to 65538  
 sfrq 100.554 fn DISPLAY 65538  
 tof 1536.3 sp -1567.1  
 tpr 61 wd 25125.6  
 pw 9.300 rfl 5538.6  
 DECOUPLER H1 lp rfp 3971.5  
 dn 0 lp -41.9  
 dof -347.2  
 dm VVY w PLOT  
 dmm w wc 250  
 dpwr 42 sc 0  
 dmf 8900 vs 109  
 nm no ph 5

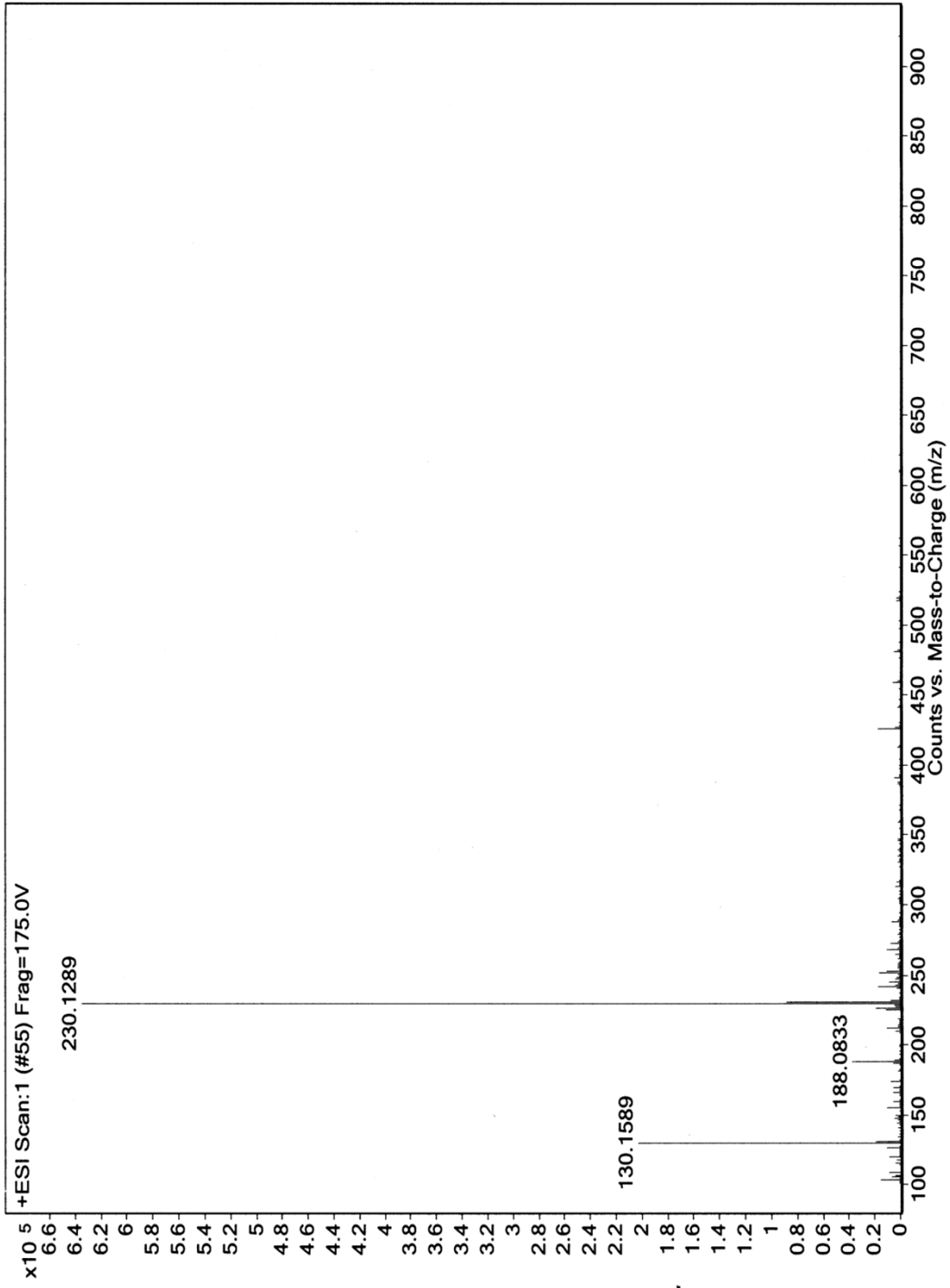


**Sample Name**  
**Inj Vol**  
**Data Filename**

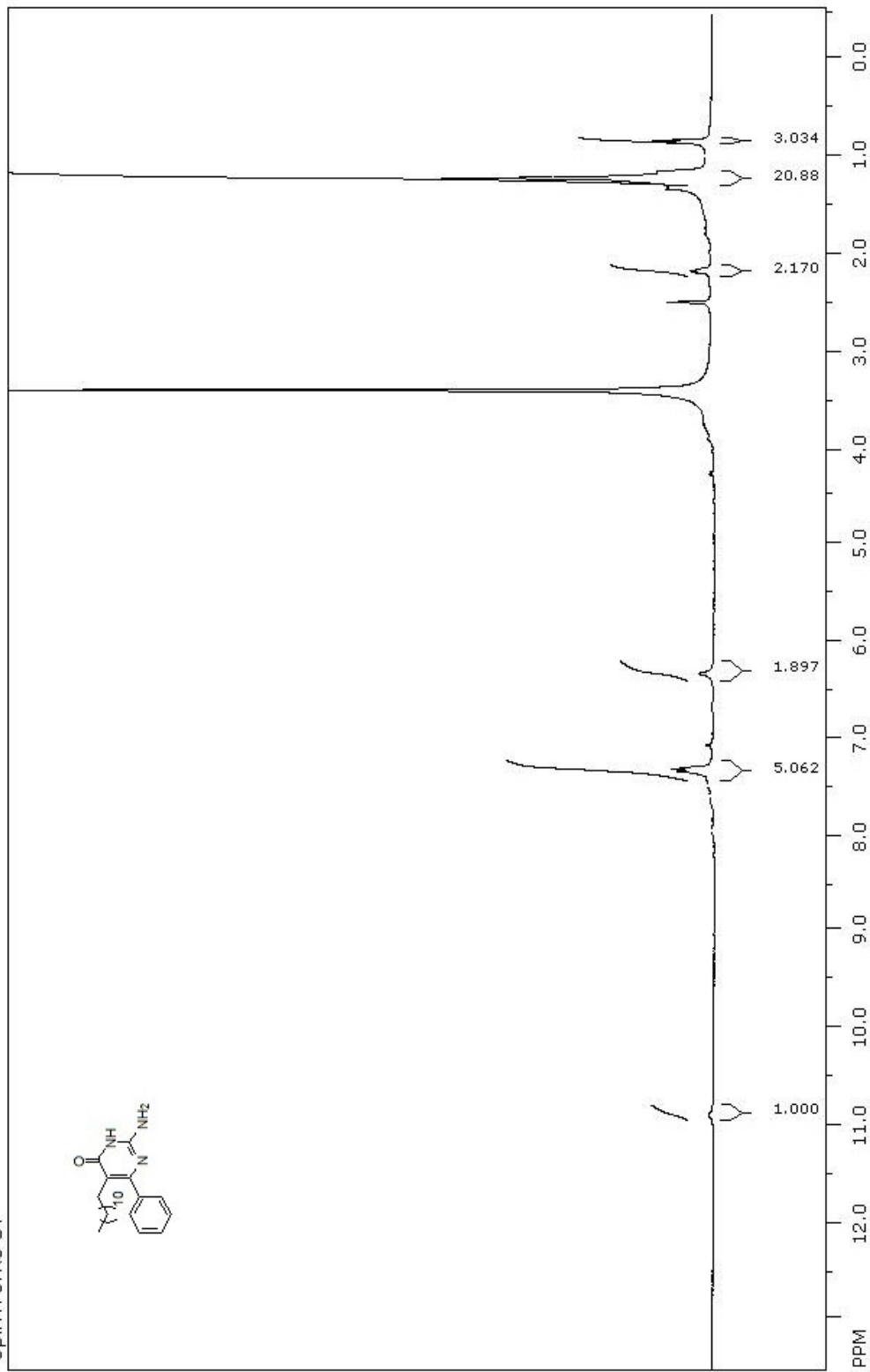
**Position**  
**InjPosition**  
**ACQ Method**

**Instrument Name**  
**Sample Type**  
**Comment**

**User Name**  
**IRM Calibration Status**  
**Acquired Time**



SpinWorks 3:



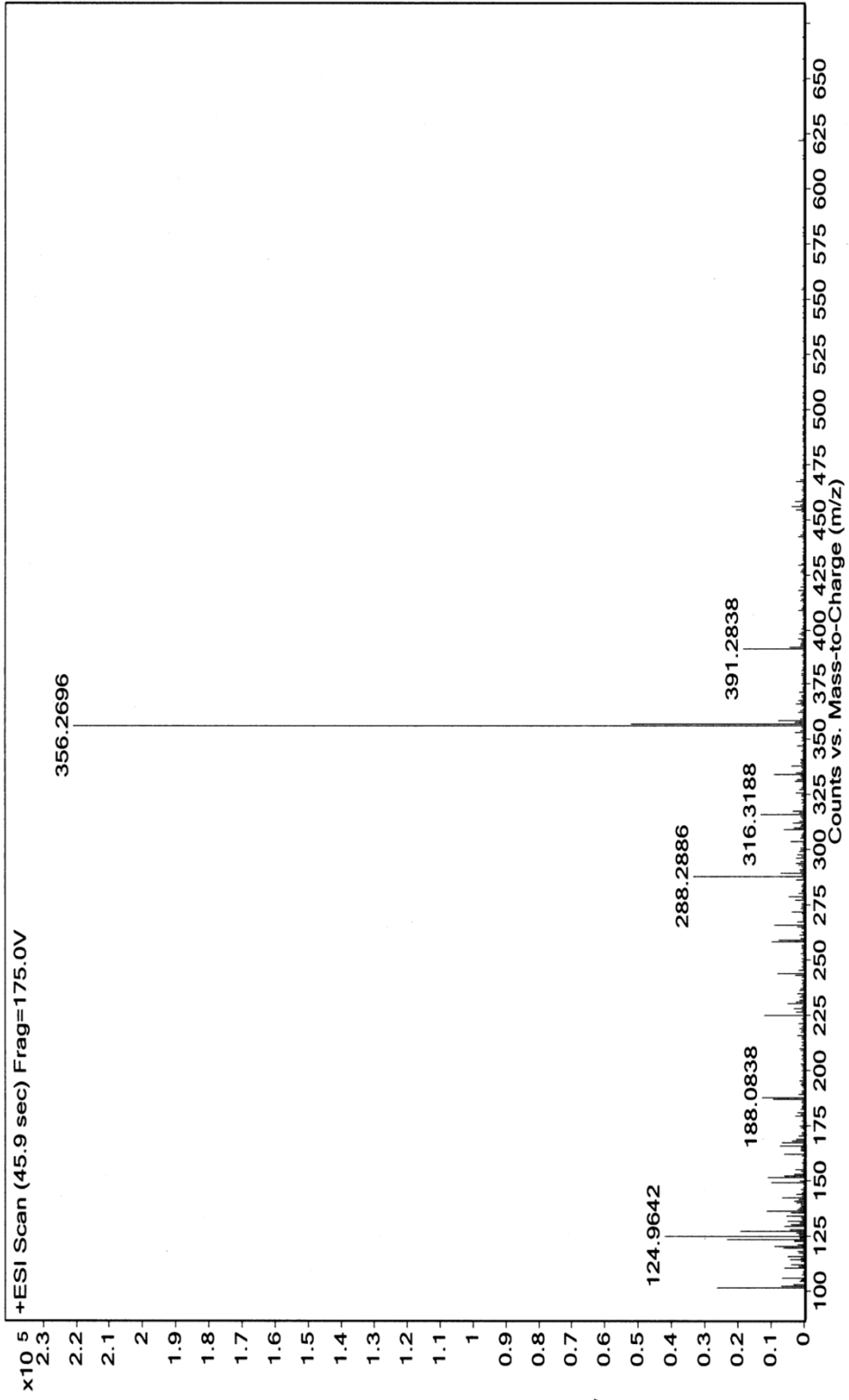
file: ...rishnan\NMR-DATA\KRK-PH-DO.fid\fid block# 1. expt: "s2pul"  
transmitter freq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32  
freq. of 0 ppm: 399.852863 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 225.006 ppm/cm: 0.56272

Sample Name  
Inj Vol  
Data Filename

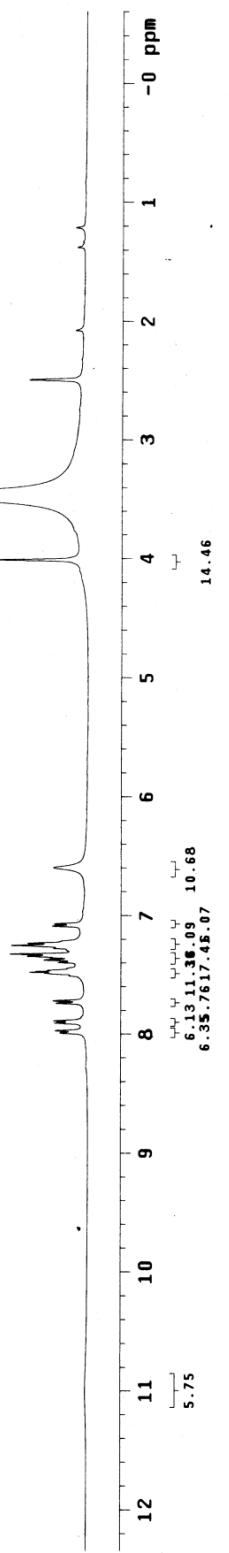
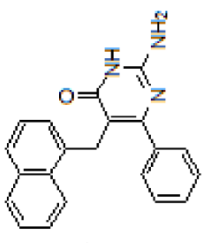
Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

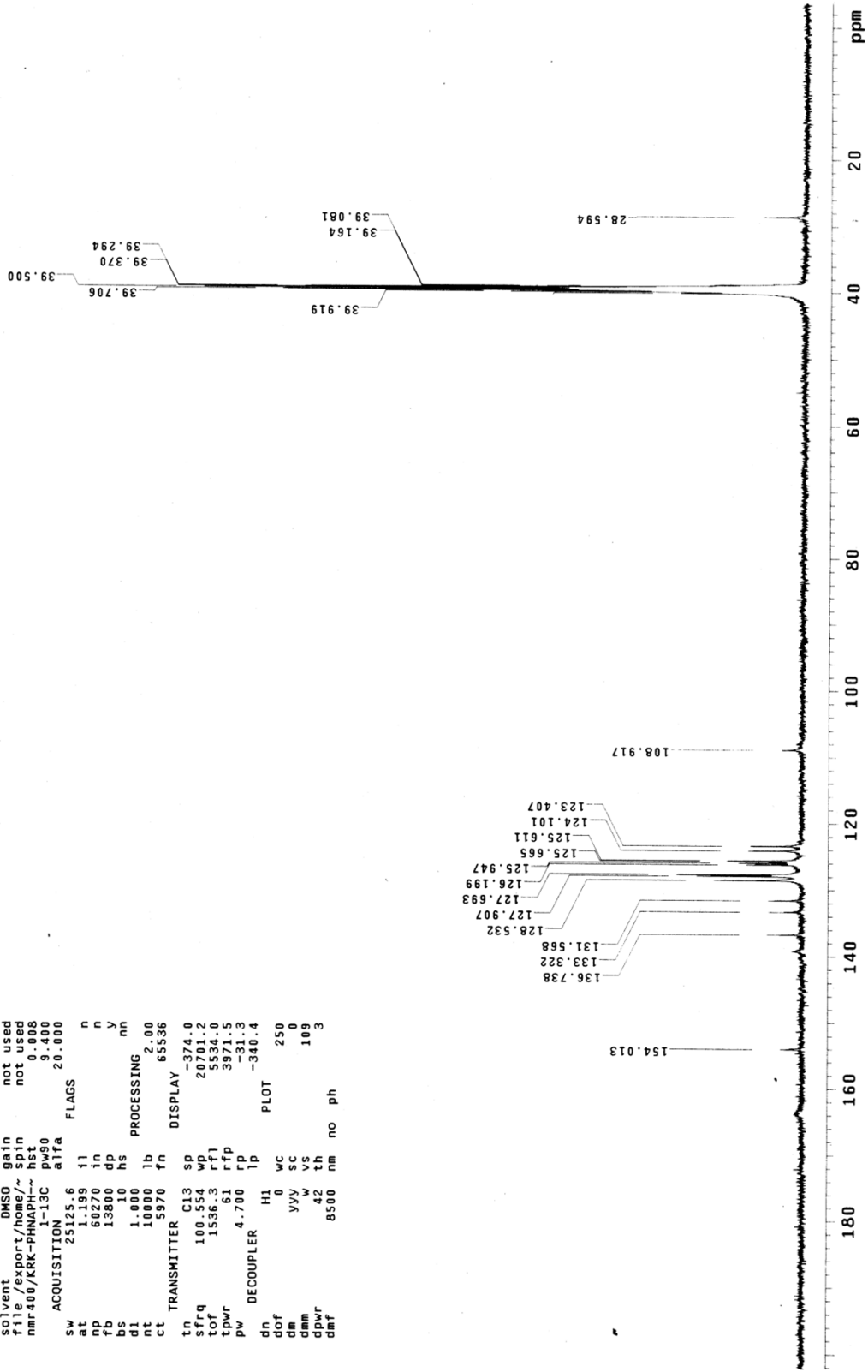
User Name  
IRM Calibration Status  
Acquired Time



SAMPLE SPECIAL  
 date Apr 28 2013 temp not used  
 solvent DMSO gain not used  
 file exp spin not used  
 ACQUISITION hst 0.008  
 sw 6389.8 pw90 15.100  
 mc 25528 a1fa 20.000  
 not used 11 n  
 bs 4 in n  
 d1 1.000 dp v  
 nt 100 hs v  
 ct 100 hs PROCESSING 0.10  
 tn TRANSMITTER lb fn 65536  
 strq 399.855 HI DISPLAY  
 tor 362.8 sp -242.9  
 dpwr 7.558 wpl 5180.5  
 pw DECOUPLER C13 rfp 1999.2  
 dn 0 lp 183.3  
 dof 0 lp -85.5  
 da nnn C PLOT  
 dnm C 250  
 dpwr 44 SC 0  
 dmf 17100 VS 269  
 nm cdc ph 42



SAMPLE date May 2 2013 SPECIAL  
 solvent DMSO gain not used  
 file /export/home/~ spin not used  
 nmr400/KKK-PHNAPH~ hst 0.008  
 1-13C pw90 9.400  
 ACQUISITION aifa 20.000  
 SW 25125.6  
 at 41.199 fl  
 pp 60270 in n  
 fb 13800 dp v  
 bs 10 hs  
 dt 1.000 lb  
 nt 10000 lb 2.00  
 ct 5970 fn 65536  
 TRANSMITTER C13 SP  
 tn -374.0  
 sfrq 100.554 wp 20701.2  
 tof 1536.3 rfl 5634.0  
 tpwr 61 rfp 3871.5  
 pw 4.700 lp -31.3  
 DECOUPLER H1 PLOT  
 dn 0 wc 250  
 dof 0  
 dm vvy sc 0  
 dnm w vs 109  
 dpwr 42 th 3  
 dnr 8500 nm no ph

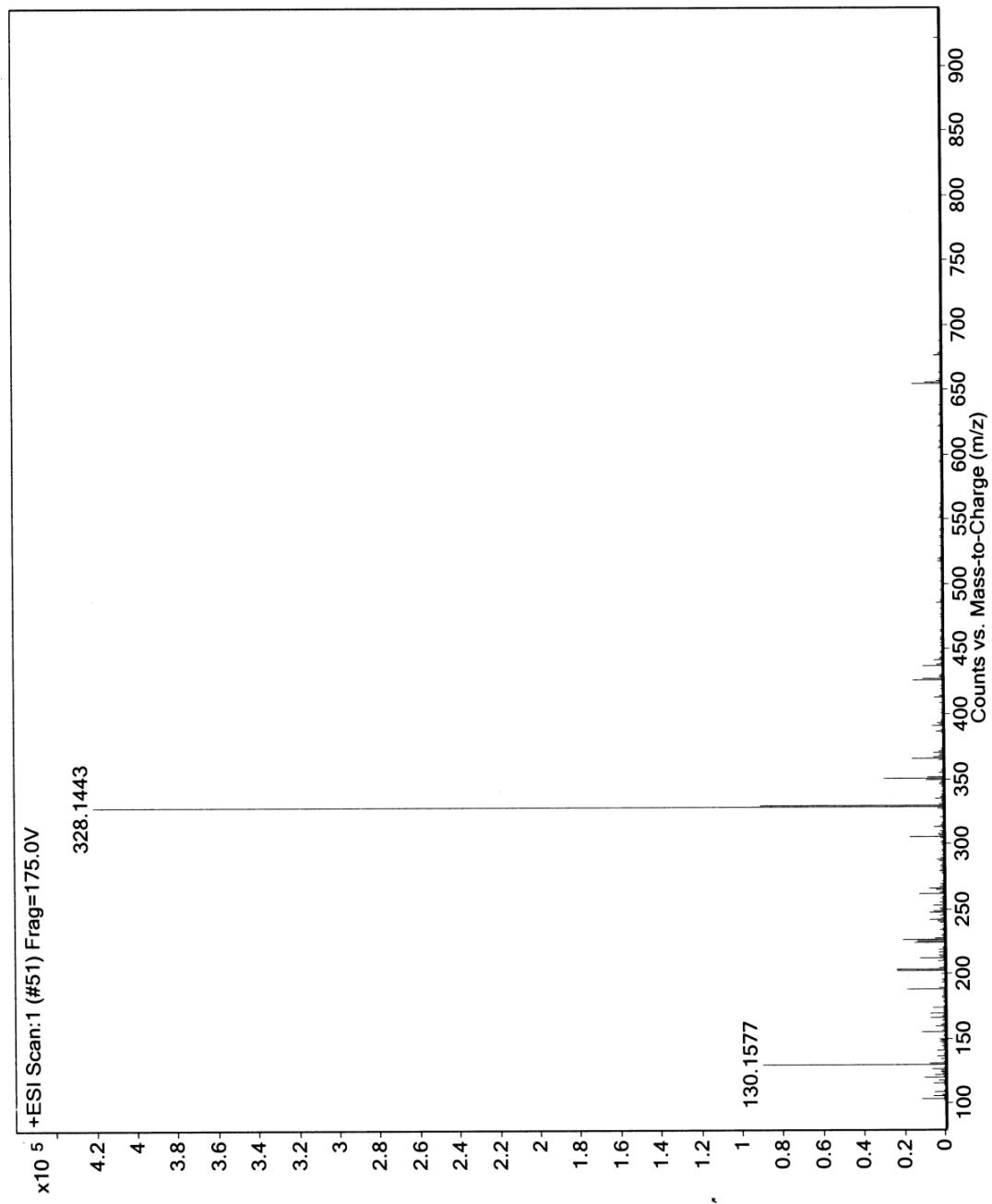


Sample Name  
Inj Vol  
Data Filename

Position  
InjPosition  
ACQ Method

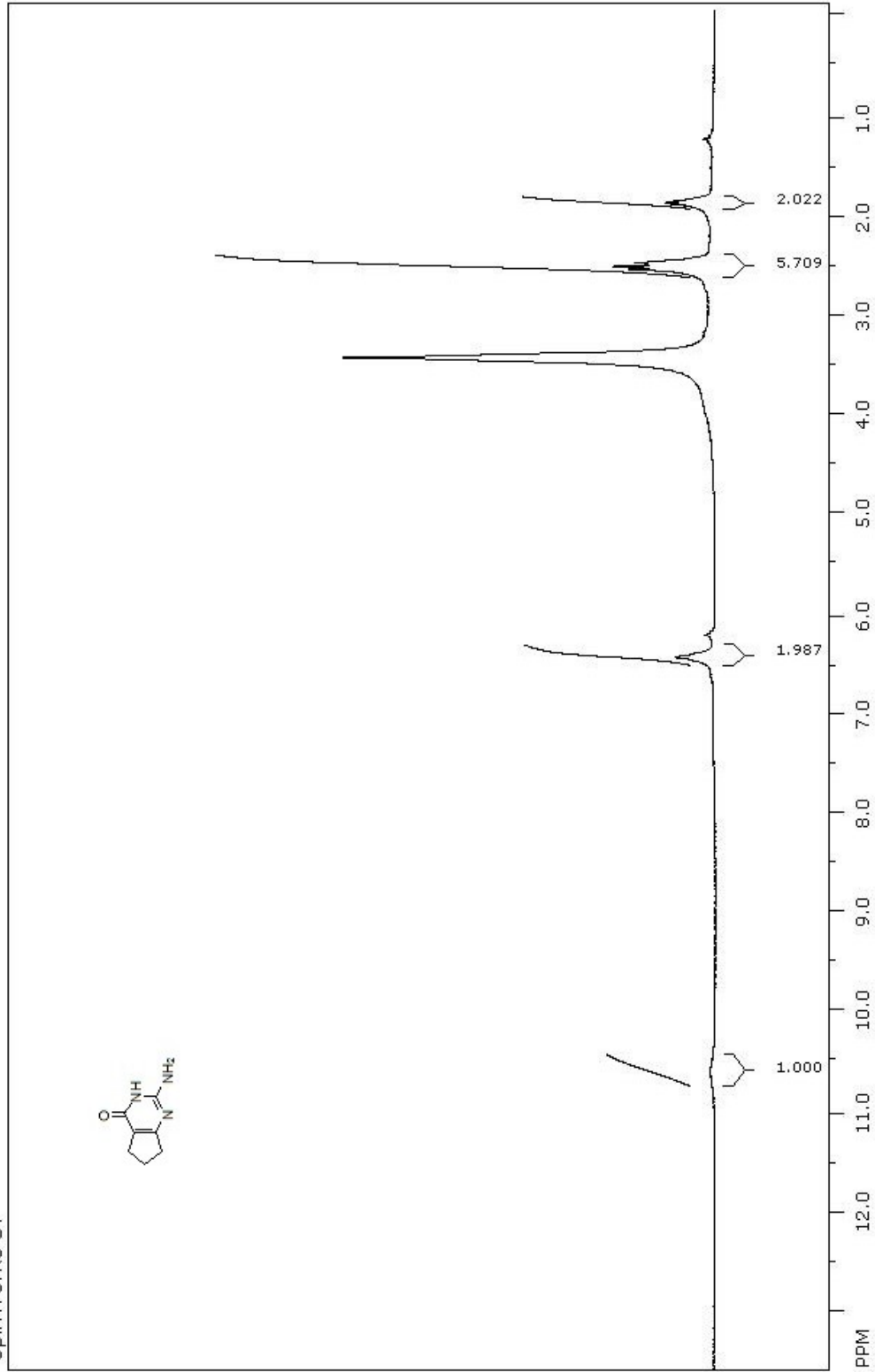
Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time



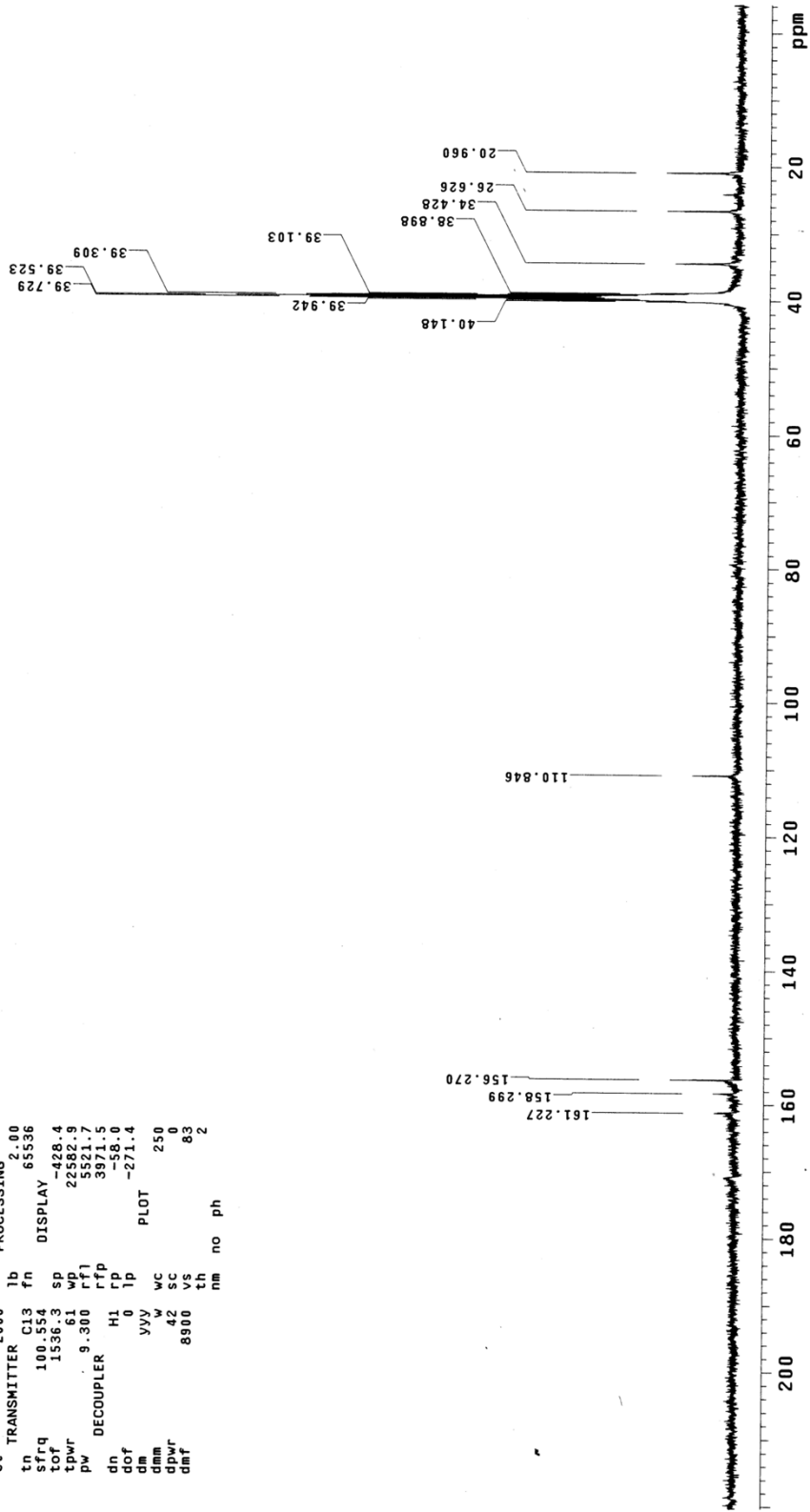


SpinWorks 3:



file: ...ishnan\NMR-DATA\KRRK-CP-GUA.fid\fid block# 1 expt: "s2pul"  
transmitter freq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32  
freq. of 0 ppm: 399.852858 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 219.746 ppm/cm: 0.54956

SAMPLE SPECIAL  
 date Jul 9 2012 temp not used  
 solvent DMSO gsin not used  
 file not used  
 ACQUISITION exp not used  
 sw 25125.6 pw90 18.600  
 at 1.199 alfa 20.000  
 np 60270 f1 n  
 fb 13800 20 in n  
 bs 20 20 in n  
 d1 1.000 dp y  
 nt 5000 hs nn  
 ct 2000  
 TRANSMITTER b 2.00  
 tn 65536  
 sfrq 100.553 tn DISPLAY -428.4  
 tof 15363 sp 2568.4  
 tdwr 61 w 5522.7  
 pw 9.300 rfl 3971.5  
 DECOUPLER H1 rfp -58.0  
 dn 0 lp -271.4  
 dof 0  
 dm yvv WC PLOT 250  
 dmm w WC 250  
 dpwr 42 SC 0  
 dmf 8900 VS 83  
 nm no ph 2

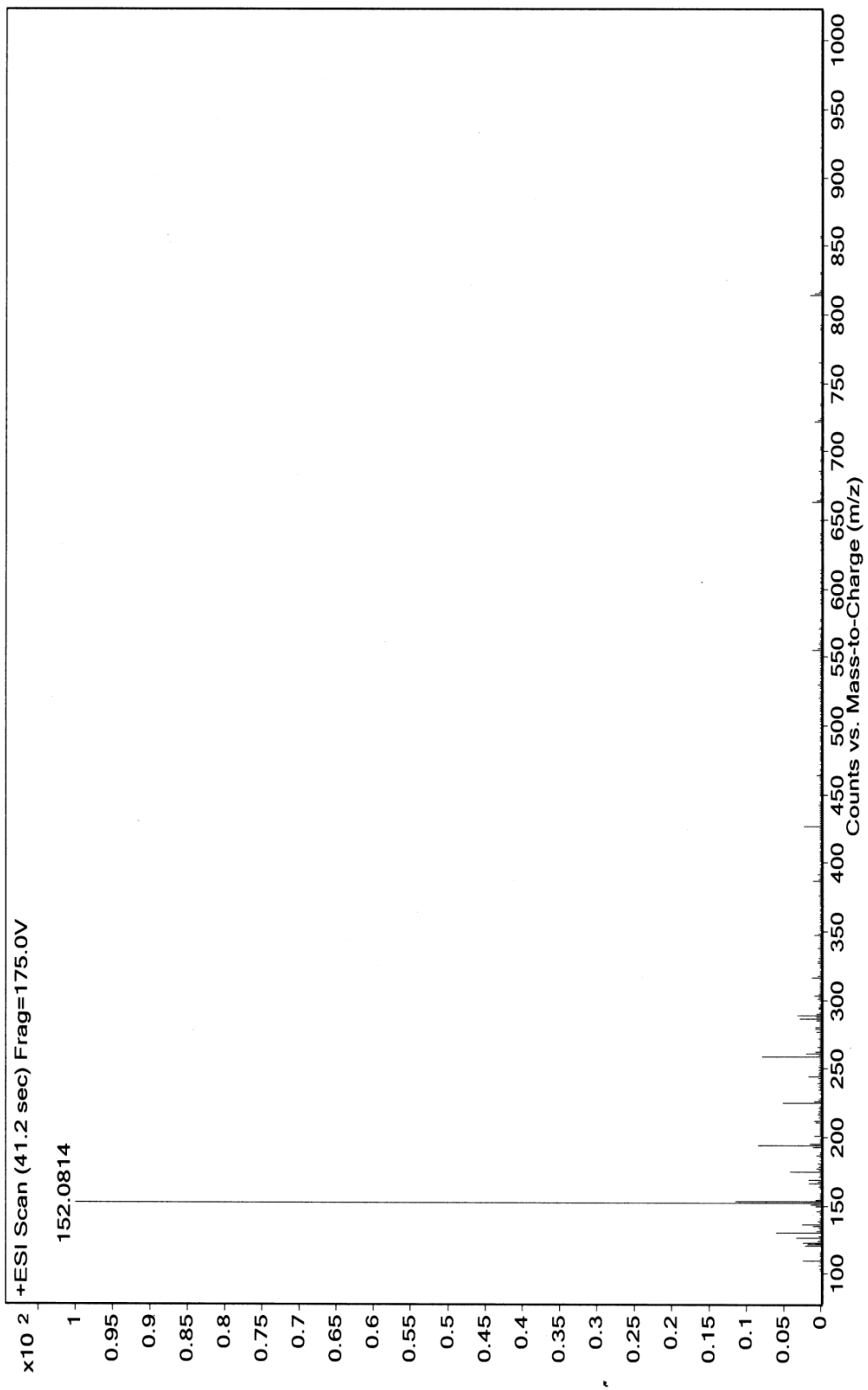


User Name  
IRM Calibration Status  
Acquired Time

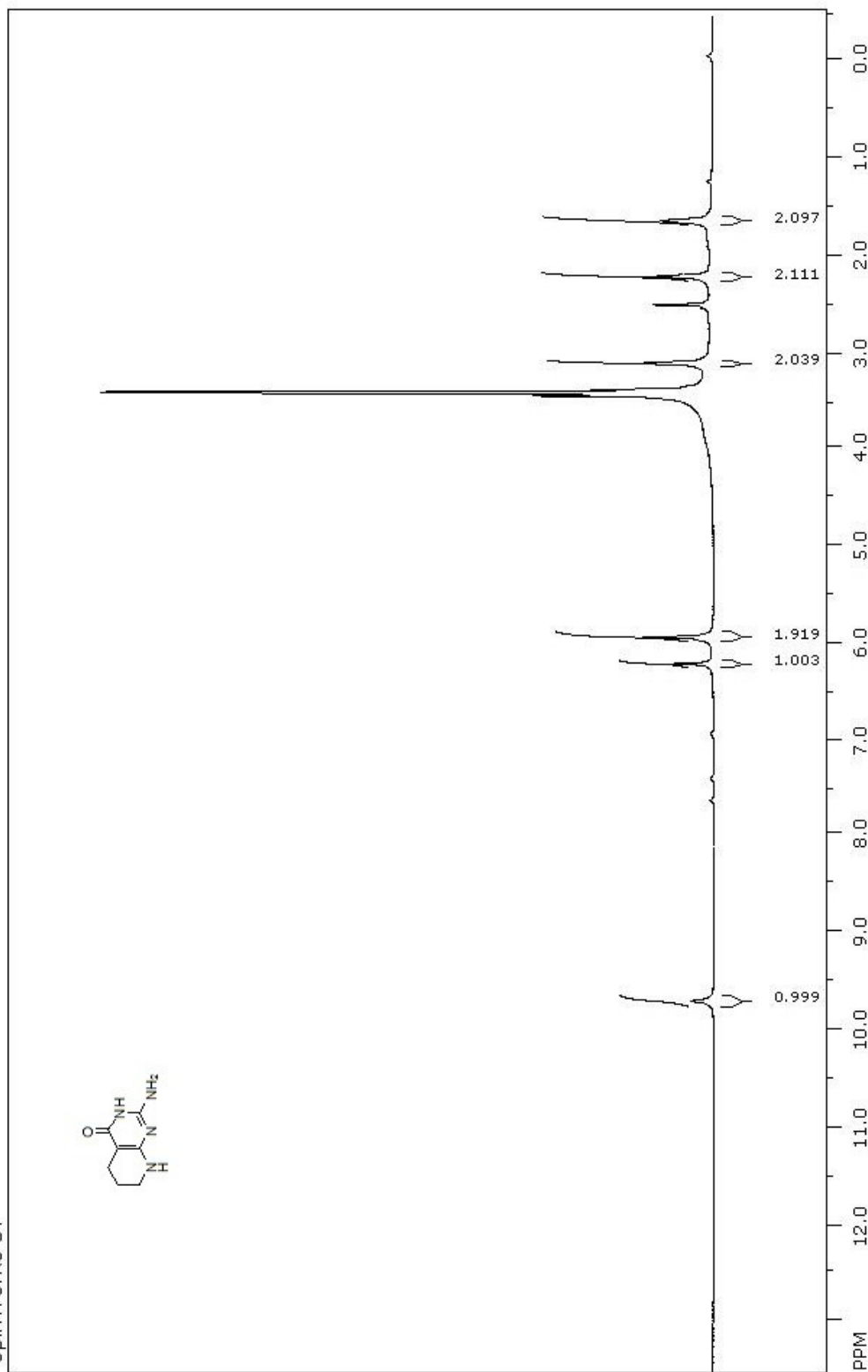
Instrument Name  
SampleType  
Comment

Position  
InjPosition  
ACQ Method

Sample Name  
Inj Vol  
Data Filename



SpinWorks 3:



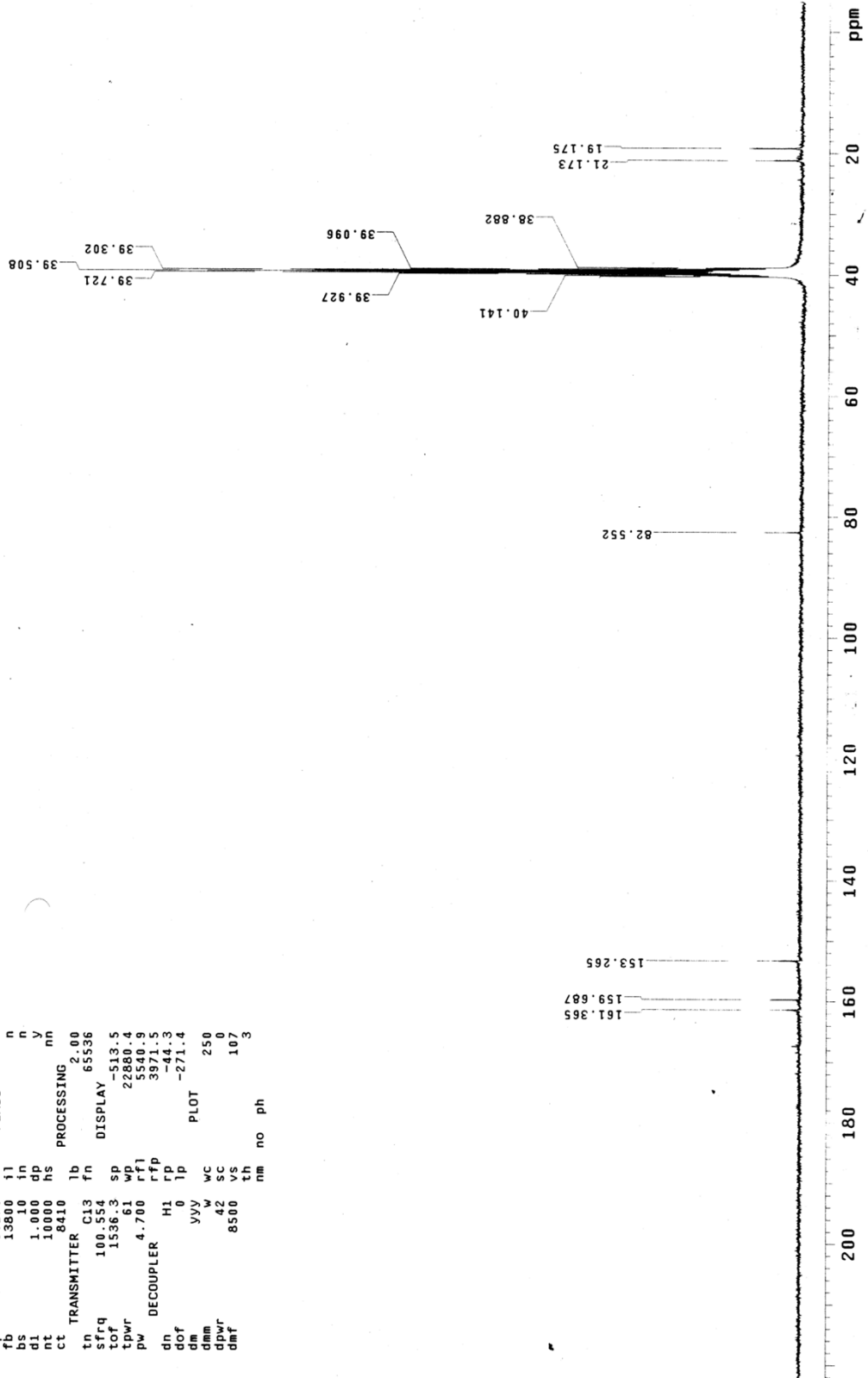
file: ...shnan\NMR-DATA\KRK-GUA-PIP.fid\fid block# 1 expt: "s2pul"  
transmitter freq.: 399.855262 MHz  
time domain size: 25528 points  
width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt  
number of scans: 32

freq. of 0 ppm: 399.852854 MHz  
processed size: 65536 complex points  
LB: 0.000 GF: 0.0000  
Hz/cm: 225.201 ppm/cm: 0.56321

KRK-PIP-GUA-13C

exp1 s2pu1

SAMPLE date May 9 2013 SPECIAL not used  
solvent DMSO gain not used  
file exp file not used  
ACQUISITION hst 0.008  
sw 25125.6 pw90 9.400  
at 1.199 alfa 20.000  
np 60270 il FLAGS  
ds 13800 il n  
bs 1.10 in n  
dl 1.000 dp n  
nt 18000 hs y  
ct 8410 lb PROCESSING 2.00  
tn TRANSMITTER C13 lb fn 65536  
sfrq 100.554 f DISPLAY -513.5  
tof 1536.3 sp 22880.4  
tavr 61 wd 5540.9  
pw DECOUPLER 4.700 rfp 3971.5  
dn 0 lp -44.3  
dof 0 lp -271.4  
dm VVY w WC 250  
dmm w SC 0  
dpwr 42 VS 107  
dmf 8500 th nm no ph 3



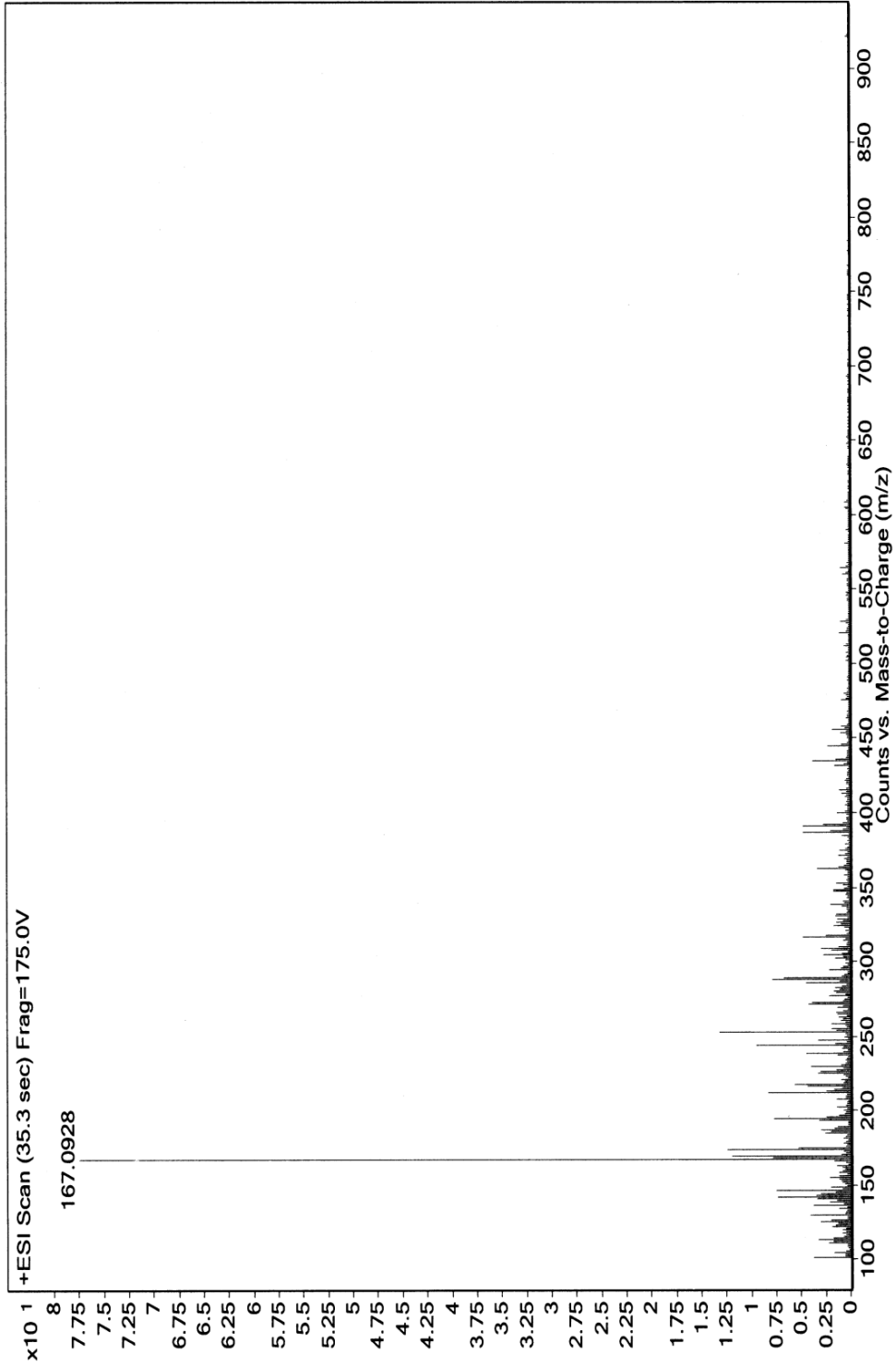
Sample Name  
Inj Vol  
Data Filename

Position  
InjPosition  
ACQ Method

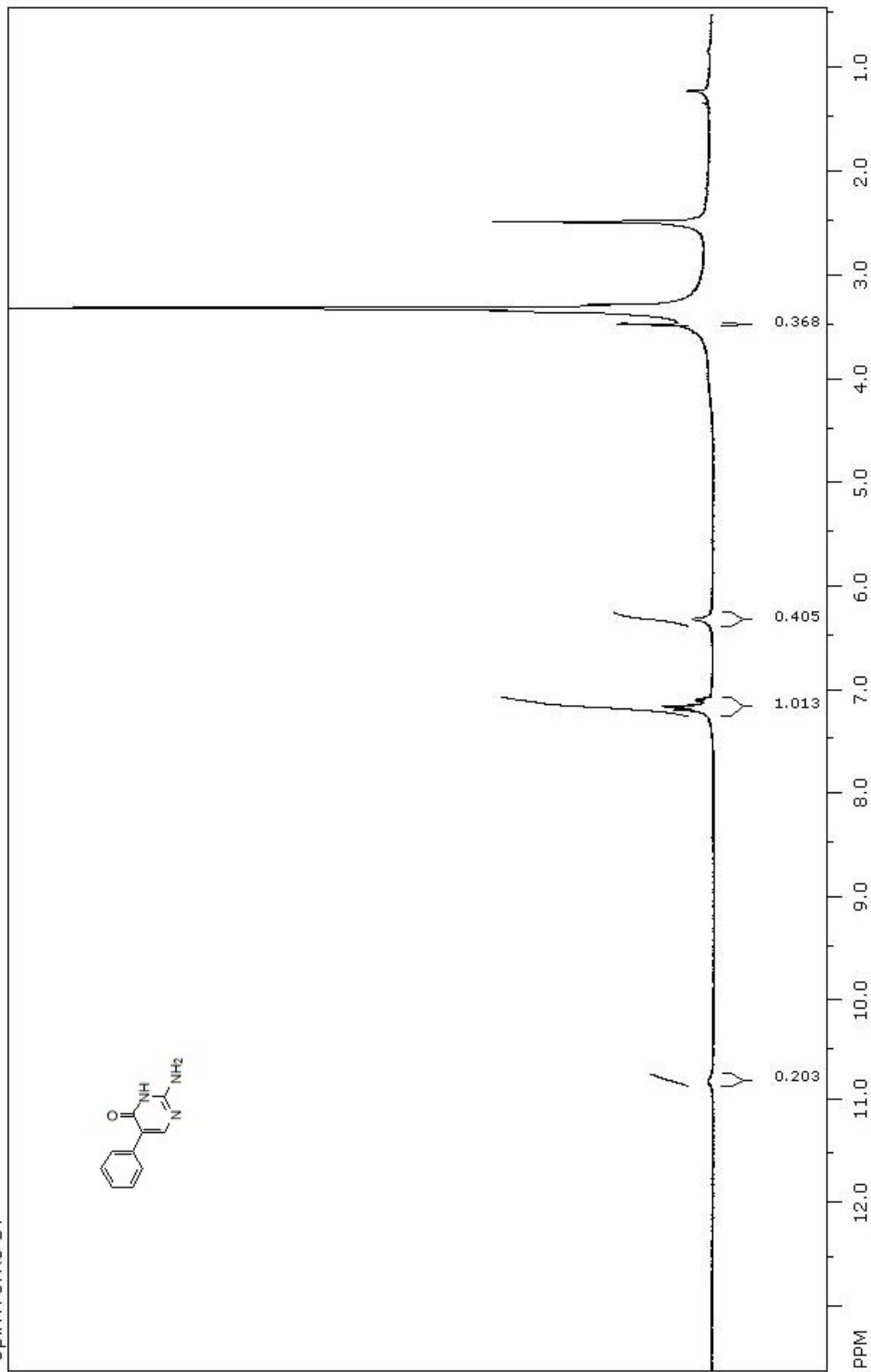
Instrument Name  
SampleType  
Comment

Instrument 1  
Sample

User Name  
IRM Calibration Status  
Acquired Time



SpinWorks 3:



file: ...ishnan\NMR-DATA\KRK-BZ-GUA.fid\fid block# 1. expt: "s2pul"

transmitterfreq.: 399.855262 MHz

time domain size: 25528 points

width: 6389.78 Hz = 15.9802 ppm = 0.250305 Hz/pt

number of scans: 32

freq. of 0 ppm: 399.852863 MHz

processed size: 65536 complex points

LB: 0.000 GF: 0.0000

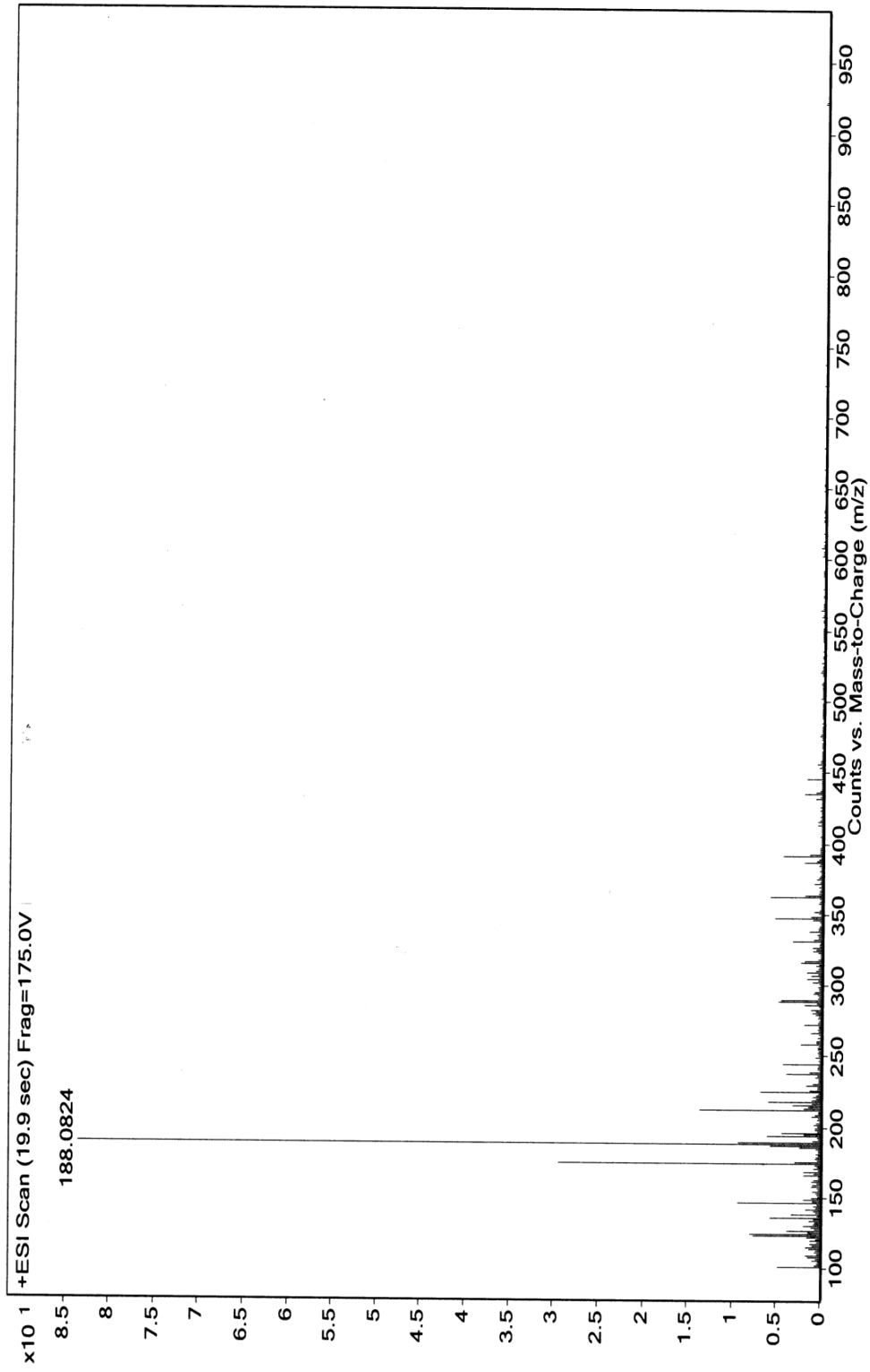
Hz/cm: 210.785 ppm/cm: 0.52715

Sample Name  
Inj Vol  
Data Filename

Position  
InjPosition  
ACQ Method

Instrument Name  
SampleType  
Comment

User Name  
IRM Calibration Status  
Acquired Time





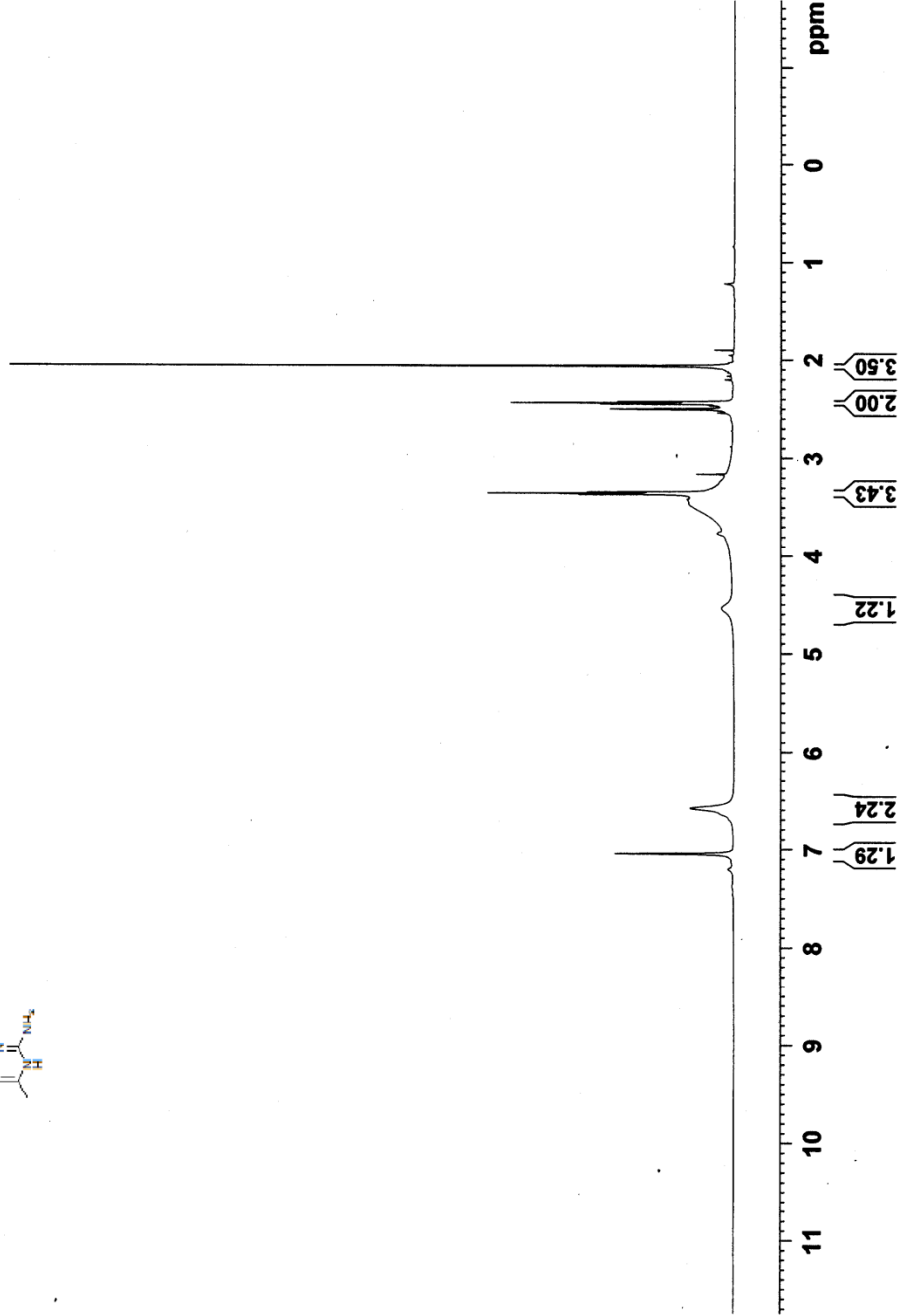
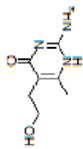


Current Data Parameters  
NAME RSK-AL-GUR-11  
EXNO  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131205  
Time 10:11  
INSTRUM spect  
PROBHD 5 mm PABBO BB  
PULPROG zg30  
TD 32768  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 12019.230 Hz  
FIDRES 0.366790 Hz  
AQ 1.3631488 sec  
RG 54.94  
DM 41.600 usec  
DE 6.50 usec  
TE 299.3 K  
FL 1.00000000 sec  
TD0 1

CHANNEL f1  
SF01 600.1737063 MHz  
NUC1 1H  
PI 12.00 usec  
PLW1 21.00000000 W

F2 - Processing Parameters  
SI 16384  
SF 600.1700054 MHz  
WDW EM  
SSB 0  
GB 0  
PC 1.00





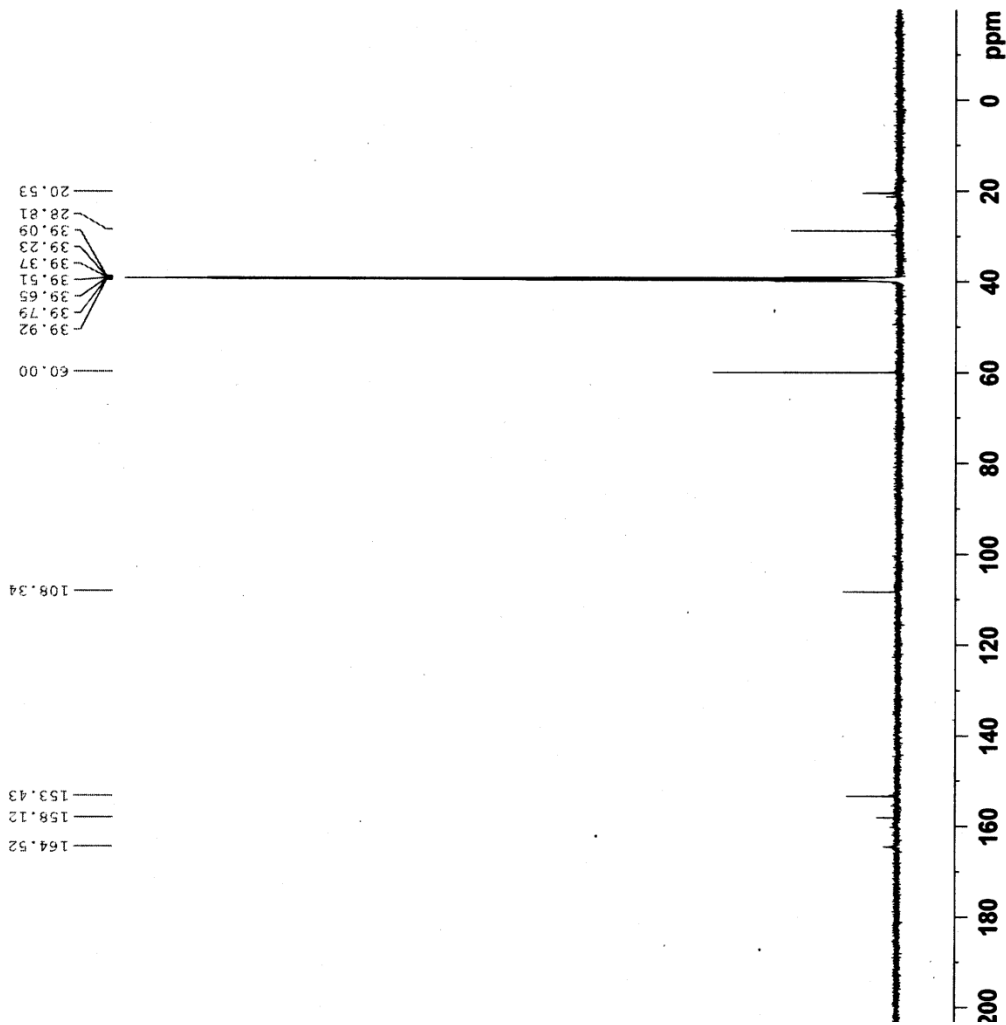
Current Data Parameters  
NAME KKK-AL-GUA-13C  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20131205  
Time\_ 10.32  
INSTRUM spect  
PROBHD 5 mm PABBO BE/  
PULPROG zgpg30  
TD 32768  
SOLVENT DMSO  
NS 239  
DS 2  
SWH 36057.691 Hz  
FIDRES 1.100393 Hz  
AQ 0.4543829 sec  
RG 65.24  
DM 13.867 usec  
DE 6.50 usec  
TE 299.3 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

==== CHANNEL f1 =====  
SFO1 150.9279571 MHz  
NUC1 13C  
P1 10.50 usec  
PLW1 95.00000000 W

==== CHANNEL f2 =====  
SFO2 600.1724007 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 70.00 usec  
PLW2 21.00000000 W  
PLW12 0.61714000 W  
PLW13 0.30239999 W

F2 - Processing parameters  
SI 16384  
SF 150.9129298 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



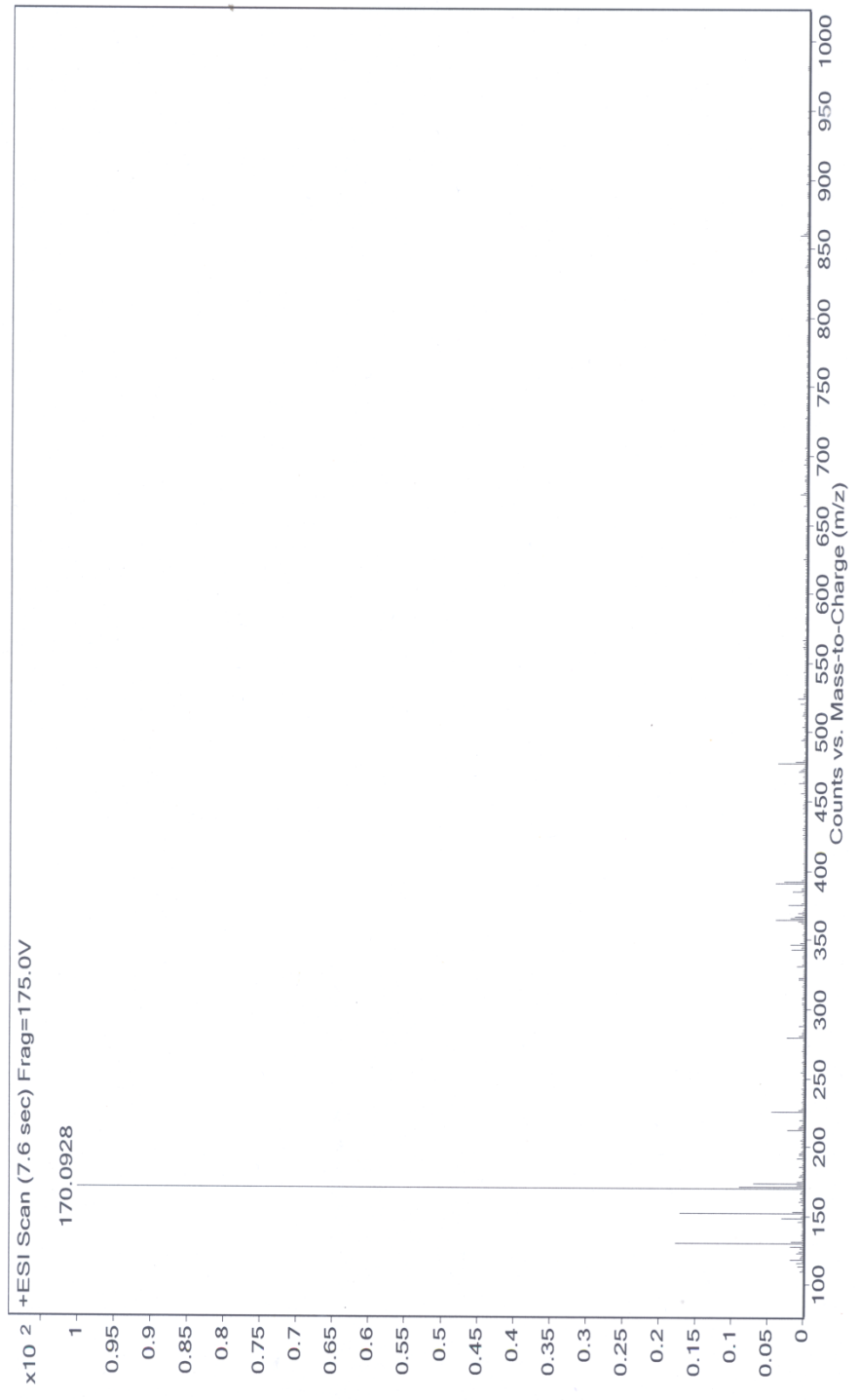
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 Inj Vol  
 Data Filename

Position  
 InjPosition  
 ACQ Method

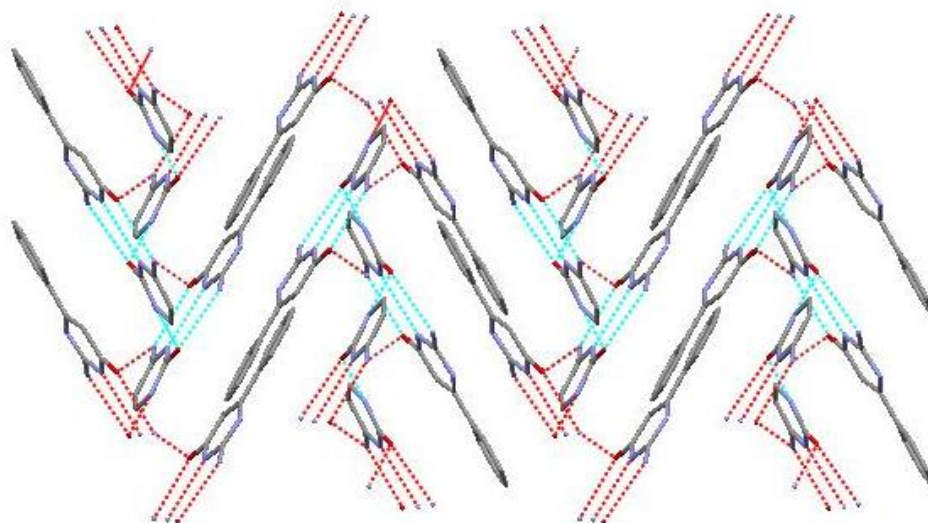
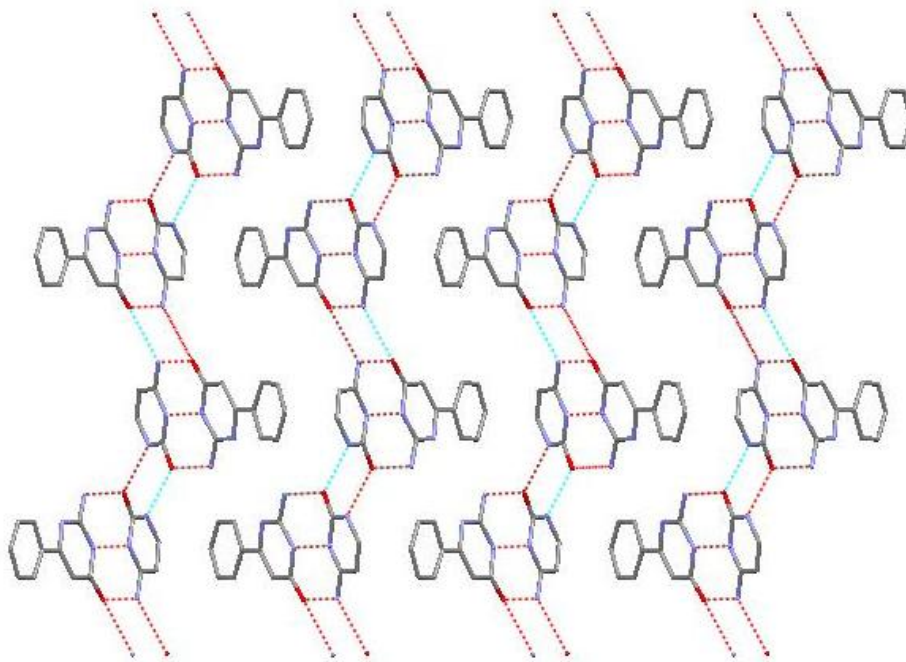
Instrument Name  
 SampleType  
 Comment

User Name  
 IRM Calibration Status  
 Acquired Time

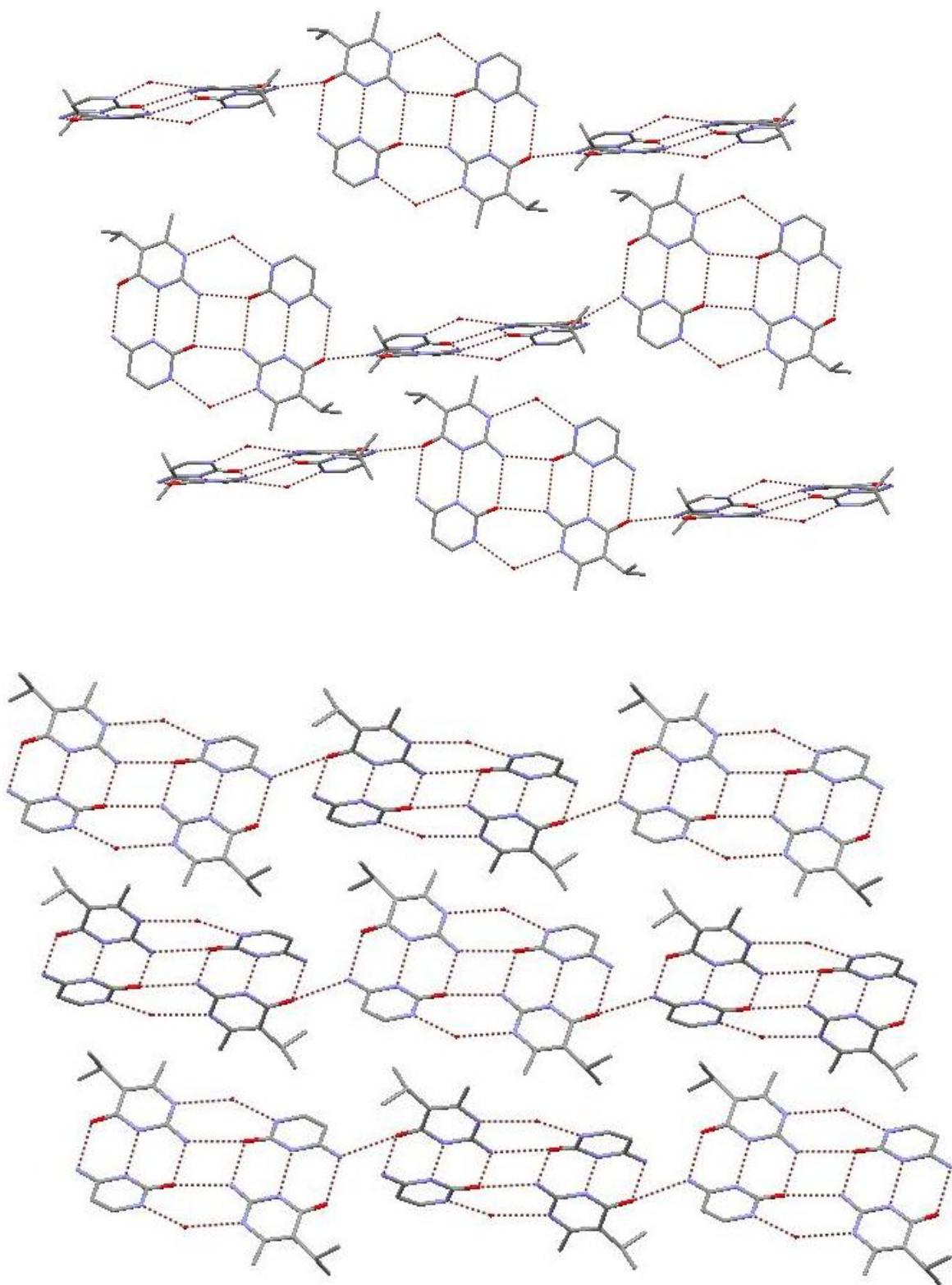
Success  
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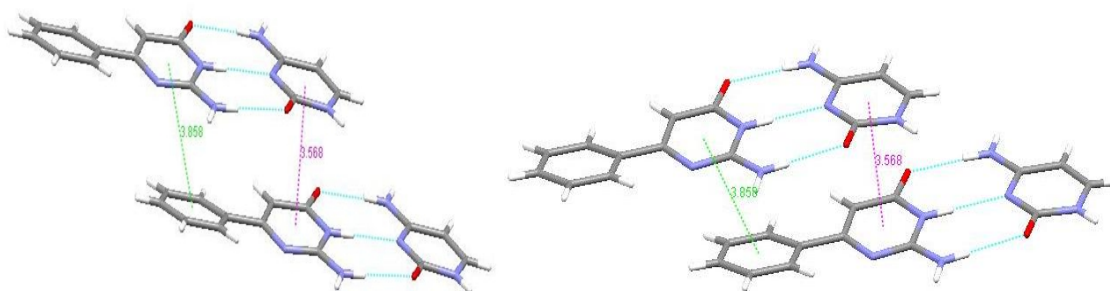
**Supramolecular structures of 6-phenyl isocytosine:cytosine co-crystal**



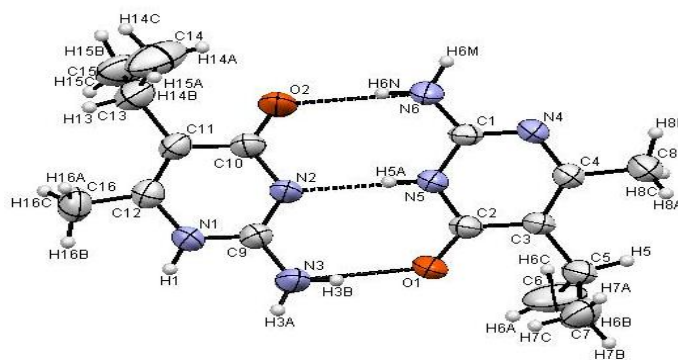
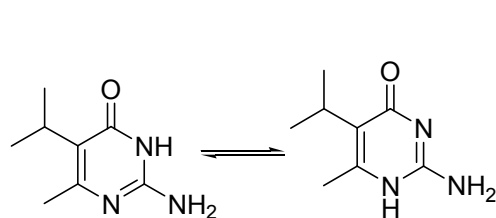
**Supramolecular structures of 5-isopropyl-6-methylisocytosine:cytosine co-crystal**



## Pi-stacking interactions



## Tautomeric forms of 5-isopropyl-6-methyl isocytosine



## Hydrogen bond distances of 6-phenyl isocytosine - cytosine co-crystal

D-H...A	D-H/Å	H...A/Å	D-H...A/Å	∠D-H...A/°	symmetry
N(1) --H(1A) ..N(4)	0.94(3)	1.94(3)	2.870(3)	177(2)	-x+1, y+1/2, -z+1/2
N(3) --H(3A) ..N(2)	0.86	2.48	3.220(2)	144	-x+1, -y+1, -z
N(3) --H(3B) ..O(2)	0.86	2.04	2.904(3)	178	-x+1, y+1/2, -z+1/2
N(5) --H(5A) ..O(2)	0.86(3)	2.05(3)	2.839(3)	152(2)	-x+1, y+1/2, -z+1/2
N(6) --H(6A) ..O(1)	0.86	1.95	2.811(3)	176	-x+1, y-1/2, -z+1/2
N(6) --H(6B) ..O(1)	0.86	1.99	2.839(3)	172	x-1, y, z

### Hydrogen bond distances of 5-isopropyl-6-methyl isocytosine -cytosine co-crystal

D-H...A	D-H/Å	H...A/Å	D-H...A/Å	∠D-H...A/°	Symmetry
N(1) --H(1A) ..O(2)	0.86	2.12	2.849(4)	143	-x+1/2, y-1/2, -z+1/2
N(1) --H(1B) ..O(2)	0.86	2.06	2.919(3)	172	x-1/2, -y-1/2, z-1/2
N(6) --H(2D) ..O(1)	0.86	2.10	2.933(3)	161	x+1/2, -y-1/2, z+1/2
N(6) --H(2E) ..O(1)	0.86	2.08	2.918(4)	166	-x,-y,-z+1
N(4) --H(20) ..O(3)	0.91(3)	1.90(3)	2.806(4)	176(3)	-x+1/2, y+1/2, -z+1/2
N(2) --H(21) ..N(5)	0.94(3)	2.02(3)	2.957(4)	179(3)	x-1/2, -y-1/2, z-1/2
O(3) --H(22) ..O(2)	0.90(4)	2.06(4)	2.944(3)	168(3)	-x+1/2, y+1/2, -z+1/2
O(3) --H(23) ..N(3)	0.87(4)	2.01(4)	2.873(4)	176(3)	

<b>6-phenyl isocytosine (5)/ cytosine co-crystal (crystallographic data)</b>	<b>CCDC # 980518</b>
Chemical formula	C14 H14 N6 O2
Formula mass	298.31
Temperature / K	296 (2)
Crystal system	Monoclinic
Space group	P21/c
a / Å	12.4798(6)
b / Å	6.8611(5)
c / Å	17.0339(10)
α / °	90.00
β / °	95.021(5)
γ / °	90.00
Unit cell volume / Å <sup>3</sup>	1452.94(15)
z	4
Final R1 value	0.0501
Final wR value	0.0856
Goodness of fit	1.096

<b>5-isopropyl-6-methyl isocytosine (6)/ cytosine co-crystal (crystallographic data)</b>	<b>CCDC # 980516</b>
Chemical formula	C12 H20 N6 O3

Formula mass	296.34
Temperature / K	296 (2)
Crystal system	Monoclinic
Space group	P21/n
a / Å	15.5249(9)
b / Å	5.5769(3)
c / Å	18.7323(11)
$\alpha$ / °	90.00
$\beta$ / °	112.714(3)
$\gamma$ / °	90.00
Unit cell volume / Å <sup>3</sup>	1496.07(15)
z	4
Final R1 value	0.0405
Final wR value	0.1109
Goodness of fit	0.876

<b>5-isopropyl-6-methyl isocytosine (6) tautomeric forms (crystallographic data)</b>	<b>CCDC # 980517</b>
Chemical formula	C16 H28 N6 O3
Formula mass	352.44
Temperature / K	296(2)
Crystal system	Monoclinic
Space group	C2/c
a / Å	19.3425(7)
b / Å	13.9961(7)
c / Å	14.4876(6)
$\alpha$ / °	90.00
$\beta$ / °	103.855(3)
$\gamma$ / °	90.00
Unit cell volume / Å <sup>3</sup>	3808.0(3)
z	8
Final R1 value	0.0438
Final wR value	0.1038
Goodness of fit	1.007